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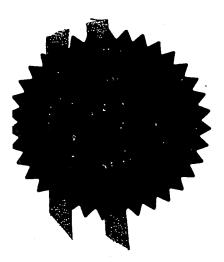
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Claims(s)

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METHODS

The present invention relates to protein kinase catalytic domain structures and mutants and screening assays making use thereof.

The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) is a key 5 protein kinase, regulating activity of a group of related protein kinases through phosphorylation. These kinases include isoforms of Protein Kinase B (also known as Akt) [Brazil and Hemmings, 2001, Scheid and Woodgett, 2001], p70 ribosomal S6 kinase (S6K) [Alessi et al., 1997, Volarevic and Thomas, 2001], p90 ribosomal S6 Kinase (RSK) [Frodin and Gammeltoft, 10 1999] and the serum and glucocorticoid induced-protein kinase (SGK) [Lang and Cohen, 2001]. These enzymes are stimulated by hormones and growth factors and phosphorylate regulatory proteins mediating the various physiological effects of these agonists.

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PDK1 possesses an N-terminal kinase catalytic domain and a C-terminal pleckstrin homology (PH) domain [Alessi et al., 1997, Stephens et al., 1998]. PDK1 activates its substrates by phosphorylating these kinases at their activation loop (reviewed in [Alessi, 2001, Toker and Newton, 2000]). The phosphorylation of PKB by PDK1 is dependent upon prior activation of the phosphoinositide 3-kinase (PI-3-kinase) and the production of the second messenger, phosphatidylinositol 3,4,5-trisphosphate (PtdIns(3,4,5)P₃) which binds to the PH domains of PDK1 and PKB. This does not activate either PKB or PDK1 but instead recruits and co-localises these enzymes at the plasma membrane.

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Unlike PKB, the other PDK1 substrates described thus far do not interact with PtdIns(3,4,5)P₃ nor is the rate at which they are phosphorylated by PDK1 further enhanced by the binding of PDK1 to PtdIns(3,4,5)P₃. Instead the ability of PDK1 to phosphorylate S6K, SGK and RSK is promoted by phosphorylation of these enzymes at a residue located C-terminal to the kinase catalytic domain in a region known as the hydrophobic motif [Alessi et al., 1997,Kobayashi and Cohen, 1999, Pullen et al., 1998]. The kinases that phosphorylate the hydrophobic motif of S6K and SGK are unknown but as the phosphorylation of this residue *in vivo* is dependent on PI-3-kinase activation, the hydrophobic motif kinases and/or the hydrophobic motif phosphatases may be regulated by PtdIns(3,4,5)P₃. In the case of RSK isoforms, phosphorylation by the ERK1/ERK2 MAP kinases induce phosphorylation of the hydrophobic motif (reviewed in Frodin and Gammeltoft, 1999).

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PDK1 belongs to the same subfamily of protein kinases as its substrates, termed the AGC protein kinases as they are related to the cAMP dependent protein kinase (PKA)/cGMP dependent protein kinase/Protein kinase C (PKC). PKA is the only AGC kinase whose crystal structure has been solved. Like all protein kinases, its catalytic core possesses an N-terminal lobe consisting mainly of β -sheet and a predominantly α -helical Cterminal lobe [Taylor et al., 1992, Husen and Kuriyan, 2002]. The ATP binding site is located in between the 2 lobes [Johnson et al., 2001, Knighton et al., 1991]. At the very C-terminus, PKA possesses an extended loop that terminates in the sequence FXXF which resembles the first part of the hydrophobic motif phosphorylation site of S6K and SGK (FXXFS/TY) in which the Ser/Thr is the phosphorylated residue [Biondi et al., 2000]. In the structure of PKA, the FXXF motif is buried in a hydrophobic pocket in the small lobe of the PKA catalytic domain [Knighton et al., 1991] and mutation of either of the Phe residues drastically reduces PKA activity towards a peptide substrate [Etchebehere et al., 1997]. Unlike other AGC kinases, PDK1 does not possess a hydrophobic motif C-terminal to its catalytic domain. However, there is evidence that PDK1 possesses a hydrophobic pocket in the small lobe of its catalytic domain similar to that

in PKA. We have biochemically demonstrated that the interaction of PDK1 with four of its substrates (S6K1, SGK1, PKζ and PKC related kinase-2 (PRK2)) is reduced or abolished by mutation of residues predicted to form part of this pocket [Balendran et al., 2000, Biondi et al., 2000]. Furthermore, mutation of a central residue in the predicted pocket, Leu 155, prevented PDK1 from phosphorylating and activating S6K1 and SGK1 without affecting its ability to phosphorylate either PKB or a short peptide substrate that encompasses the activation loop of PKB (T308tide) [Biondi et al., 2000]. The hydrophobic pocket on the kinase domain of PDK1 has been termed the "PIF-pocket" after the name of the first AGC-kinase hydrophobic motif-containing peptide (PDK1 Interacting Fragment) that was found to bind PDK1 [Balendran et al., 1999a]. It has been suggested that the PIF-pocket in PDK1 functions as a docking site, enabling PDK1 to interact with some of its.physiological substrates. Furthermore, there is evidence that phosphorylation of the hydrophobic motif of S6K1, SGK and RSK2 [Balendran et al., 1999b, Biondi et al., 2001, Frodin et al., 2000] promotes the interaction of these enzymes with PDK1. These findings suggest that the PIF-pocket on PDK1 could contain a phosphate binding site promoting the binding of PDK1 to a subset of substrates (S6K, SGK and RSK) once these enzymes have been phosphorylated at their hydrophobic motif. This would result in a physiological phosphate dependent interaction. In addition there is evidence that occupancy of the PIF-pocket activates PDK1 as peptides that encompass the hydrophobic motif of PRK2 [Biondi et al., 2000] and RSK [Frodin et al., 2000] induce a 4-6-fold activation of PDK1.

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Previous predicted structures PDK1 catalytic domain were obtained using homology modelling methods based upon structural information available from the catalytic domain of PKA (Biondi et al., 2000). These predictions of the PDK1 catalytic domain structure were thus biased towards the catalytic domain from which the structural information was obtained.

We have determined a crystal structure for the kinase domain of the AGC family protein kinase PDK. The structure defines the PIF-pocket and reveals an adjacent possible phosphate binding site. Furthermore, we have performed structure-based mutagenesis and biochemical analysis which support the existence of such a phosphate-binding site. This may mediate the phosphate dependent docking interaction with substrates such as (for PDK1) S6K and SGK. We have used a novel algorithm to define the conformational state of the crystallised PDK1 relative to all the reported structures of PKA, which shows that while PDK1 has all the signs of being in an active form in the crystal, its overall conformation is in-between and 'open' and 'closed' state. On the basis of this work we provide drug screening methods and mutated protein kinase molecules (which are useful in, for example, drug screening methods).

A first aspect of the invention provides a method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

The term PDK1 as used herein includes a polypeptide (a PDK1 polypeptide) comprising the amino acid sequence identified as PDK1 in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776-789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714, or a variant, fragment, fusion or derivative thereof, or a fusion of a said variant or fragment or derivative, for example as described in WO98/41638, incorporated herein by reference. It is preferred that the said PDK1 polypeptide is a protein kinase. It is preferred that the said PDK1 polypeptide is a protein kinase that is capable of phosphorylating a threonine residue that lies in a Thr-Phe-Cys-Gly-Thr-10 Xaa-Glu-Leu consensus motif (where the underlined Thr corresponds to the threonine that is phosphorylated by PDK1 and Xaa is a variable residue), and preferably that is capable of phosphorylating PKB, for example PKBa, at residue Thr308. The rate at which the said PDK1 polypeptide is capable of phosphorylating a threonine residue as described above may be increased 15 in the presence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂ but it will be appreciated that this is not essential. The said polypeptide may be capable of phosphorylating the equivalent residues to Thr308 of PKBa on PKC isoforms (LeGood et al (1998) Science 281: 2042-2045; et al (1998) Curr. Biol. 8: 1069-1077; Dutil et al (1998) Curr. Biol. 8:1366-1375), p70 S6 20 kinase (Alessi et al (1998) Curr. Biol. 8: 69-81; Pullen et al (1998) Science 279, 707-710), SGK (sequence given in Webster et al (1993) Mol. Cell. Biol. 13, 1031-2040; equivalent residues identified in US application no 112217 filed on 14 December 1998; GB 9919676.8, filed on 19 August 1999, and Kobayashi & Cohen (1999)) and PKA (Cheng et al (1998) Proc. 25 Natl. Acad. Sci. USA 95: 9849-9854). It may further be preferred that the substrate specificity and/or other characteristics of the said PDK1 polypeptide in vitro may be substantially as reported in Alessi D.R et al (1997) Curr. Biol. 7: 261-269, Alessi D.R et al (1997) Curr. Biol. 7: 776789, Stokoe D et al (1997) Science 277: 567-570 or Stephens L et al (1998) Science 279: 710-714.

We have found that a fragment of PDK1 consisting essentially of residues equivalent to residues 51 to 359 of full length human PDK1 is particularly beneficial for determining a structure for the catalytic domain of PDK1. This fragment has, for example, protein kinase activity and surprisingly beneficial solubility and stability characteristics which make it particularly suitable for structural studies, for example formation of crystals which may be analysed by X-ray crystallography methods. Other fragments of PDK1 were surprisingly found to be unsuitable for crystallisation, as discussed in Example 5.

It is particularly preferred that the structure is one determined for the fragment consisting of residues 51 to 359 of full length human PDK1. The fragment may comprise an N-terminal or C-terminal fusion polypeptide (ie amino acid sequence not derived from PDK1), though this is preferably of less than or equal to about 10, 5, 4, 3, 2 or 1 amino acids. For example, it is particularly preferred that the structure is one determined for a polypeptide consisting residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro (or less preferably other sequence forming part of a protease cleavage site) preceding the methionine corresponding to Met51 of human PDK1. A further preferred structure is one determined for the fragment consisting essentially of residues 71 to 359 of full length human PDK1 (or residues equivalent thereto), which also has protein kinase activity.

It is particularly preferred that the structure is one determinable by a method as described in Example 1, for example a structure obtainable by X-ray analysis from a crystal obtainable using a mother liquor solution comprising

ammonium sulphate, preferably between 1.8 and 2.2M. It is particularly preferred that the mother liquor solution is of pH 7 to 9, preferably 7 to 8.5, most preferably pH8.5, and comprises ammonium sulphate and preferably ATP. Crystals may form in the absence of ATP but better crystals may be obtained in the presence of ATP. Preferably the crystal is obtainable using a mother liquor solution containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP. Further preferred details of the crystallisation and X-ray analysis are described in Example 1, for example as partially summarised in Table 1 (shown in Example 1).

It is particularly preferred that the structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure based or modelled on such a structure or co-ordinates. The co-ordinates shown in Example 2 are for the PDK1 fragment with all alternate side chains. The co-ordinates shown in Example 3 are for the PDK1 fragment without alternate side chains. The co-ordinates shown in Example 4 are for the dimer of the PDK1 fragment, without alternate side chains; chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

It is preferred that the molecule is predicted to bind to a region of the structure termed the "PIF binding pocket", the "phosphate binding pocket" and/or the α C helix (residues equivalent to 123-136 of full length human PDK1), particularly the residue equivalent to Arg 131 of full length human PDK1, or interacting regions. As discussed in Example 1, the PIF binding pocket is considered to be formed by residues including Lys115, Ile118, Ile119 on the α B helix, Val124, Val127 on the α C helix and Leu 155 on β -sheet 5. The phosphate binding pocket is considered to be formed by residues including Lys76, Arg 131, Thr 148 and Gln150. Residues of the α C helix that are considered to interact either with phosphate bound in the

phosphate binding site or intermolecularly with phosphorylated Ser241 of PDK1 include Arg131 (phosphate binding site) and Arg 129 and His126 (phosphorylated Ser241). Glu 130 is involved in binding the α-phosphate of the bound ATP, and Val124 and Val127 form part of the PIF binding pocket, as discussed in Example 1.

It is preferred that the compound is for modulating the protein kinase activity of PDK1. The protein kinase activity of PDK1 that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu ("PDK1" activity). Alternatively or in addition, the modulated activity may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Phe-Xaa-Xaa-Phe-Ser/Thr-Phe/Tyr ("PDK2" activity). The substrate polypeptide may be, for example, a PKB, SGK, p70 S6 kinase, PKC or (in relation only to phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Thr/Ser-Phe-Cys-Gly-Thr-Xaa-Glu-Leu) PKA polypeptide. The modulated protein kinase activity may be towards PKB or other PH-domain-comprising/phosphoinositide-binding substrate of PDK1; or SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY; or an artificial substrate such as T308tide (which comprises the sequence of PKB which is phosphorylated by PDK1) or PDKtide (which comprises the sequence of PKB which is phosphorylated by PDK1 (eg T308tide) fused to a sequence mimicking a phosphorylated hydrophobic motif ie FXXFZY, in which Z is a negatively charged (for example acidic) residue (eg PIFtide)). substrates for PDK1 are discussed, for example, in WO 01/44497. Other activities of PDK1 that may be modulated include interactions with other polypeptides or phosphoinositides and/or intramolecular interactions.

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It is preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of the PDK1 is a three-dimensional structure of at least a part of the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, and a compound that is predicted to interact with the said PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1 is selected. Alternatively, the compound may bind to a portion of said PDK1 polypeptide that is not the PIF binding pocket, the phosphate binding pocket and/or the α C helix, or interacting regions of PDK1, for example so as to interfere with the binding of the ATP or substrate polypeptide or their access to the catalytic site. In a still further example, the compound may bind to a portion of PDK1 so as to decrease said polypeptide's activity by an allosteric effect. This allosteric effect may be an allosteric effect that is involved in the natural regulation of PDK1's activity.

It is further preferred that the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure of the part of the protein kinase catalytic domain of PDK1 that is defined by residues Lys115, Ile118, Ile119 (on the αB helix), Val124, Val127 (on the αC helix) and Leu 155 (on β -sheet 50 and/or residues Lys76, Arg 131, Thr 148 and Gln150 and/or residues Arg131, Arg 129, His126, Glu 130 of full-length human PDK1 and a compound that is predicted to interact with the said part of the protein kinase catalytic domain is selected.

For example, it is preferred if the portions of the structure of PDK1 shown in Figures 1 and 2 as forming the PIF binding pocket and/or phosphate binding pocket and/or α C helix interactions (for example with

phosphoserine241) are compared with the structure of the candidate compound.

A further aspect of the invention provides a method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Vall27 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase. wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or a helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally also the hydrophobic pocket and/or aC helix or region interacting therewith, is selected.

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The three-dimensional structure of a compound may be compared with the three-dimensional structure of the hydrophobic and/or phosphate binding pocket and/or αC helix or region interacting therewith, as appropriate. A compound that can interact with the hydrophobic pocket and/or phosphate binding pocket, in particular residues noted above as defining such regions, in a similar manner (for example similar separation and/or type of interaction ie hydrophobic or ionic, and/or similar cumulative energy of interaction) to an interacting polypeptide such as S6K-pHM may be

selected. Methods of assessing the interaction are well known to those skilled in the art and are discussed further below.

The three-dimensional structures that are compared may be, as appropriate, predicted or modelled three-dimensional structures (for example on the basis of a PDK1 structure as referred to above, for example as represented by the co-ordinates given in Examples 2, 3 or 4) or may be three-dimensional structures that have been determined, for example by techniques such as X-ray crystallography, as well known to those skilled in the art. The three-dimensional structures may be displayed by a computer in a two-dimensional form, for example on a computer screen. The comparison may be performed using such two-dimensional displays.

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The following relate to molecular modelling techniques: Blundell et al (1996) Stucture-based drug design Nature 384, 23-26; Bohm (1996) Computational tools for structure-based ligand design Prog Biophys Mol Biol 66(3), 197-210; Cohen et al (1990) J Med Chem 33, 883-894; Navia et al (1992) Curr Opin Struct Biol 2, 202-210.

The following computer programs, for example, may be useful in carrying out the method of this aspect of the invention: GRID (Goodford (1985) J Med Chem 28, 849-857; available from Oxford University, Oxford, UK); MCSS (Miranker et al (1991) Proteins: Structure, Function and Genetics 11, 29-34; available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell et al (1990) Proteins: Structure, Function and Genetics 8, 195-202; available from Scripps Research Institute, La Jolla, CA); DOCK (Kuntz et al (1982) J Mol Biol 161, 269-288; available from the University of California, San Francisco, CA); LUDI (Bohm (1992) J Comp Aid Molec Design 6, 61-78; available from Biosym Technologies, San Diego, CA); LEGEND (Nishibata et al (1991) Tetrahedron 47, 8985;

available from Molecular Simulations, Burlington, MA); LeapFrog (available from Tripos Associates, St Louis, MO); Gaussian 92, for example revision C (MJ Frisch, Gaussian, Inc., Pittsburgh, PA ©1992); AMBER, version 4.0 (PA Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA ©1994). Programs may be run on, for example, a Silicon GraphicsTM workstation, Indigo²TM or IBM RISC/6000TM workstation model 550.

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Several *in silico* methods could be employed, for example, via a substructure search for new ligands using programmes such as CHEM DRAW or CHEM FINDER. The basic structure of the natural ligand (for example a phosphorylated hydrophobic motif peptide such as S6K-pHM) capable of binding to PDK1 (or other protein kinase) is taken (or predicted) and various structural features of it (for example the hydrophobic and negatively charged entities) are submitted to a programme which will searches a set of chemical company catalogues for chemicals containing this substructure.

These compounds are then screened by eye for groups that could not interact with the PIF/phosphate binding pockets (or the αC residues/interacting region) because, for example, they are too large or have steric or charge hindrance, and those are discarded. The remaining chemicals are submitted to a PRODRG server and topologies/co-ordinates for these chemicals are created. These chemicals are modelled into the structure, from which chemicals that are possibly able to bind to the PIF/phosphate binding site domain/αC helix/interacting region are selected. Further details of the PRODRG programme are available at http://davapc1.bioch.dundee.ac.uk/programs/prodrg/prodrg.html.

These compounds may then be ordered or synthesised and assessed, for one or more of ability to bind to and/or modulate PDK1 (or other protein kinase) activity. The compounds may be crystallised with the PDK1 or other protein kinase protein and the structure of any complex determined.

An alternative approach is to use PRODRG: a tool for generating GROMOS/MOL2/WHATIF topologies and hydrogen atom positions from small molecule PDB files. We take the natural ligand and computationally vary all possible groups at each site on the ligand, with a variety of new groups while the protein co-ordinates and the ligand back-bone co-ordinates remain fixed the results can then be screened for hindrance and repulsion, and the molecules are obtained either through catalogues or made.

As noted above, the selected or designed compound may be synthesised (if not already synthesised) or purified and tested for its effect on the relevant hydrophobic/phosphate pocket-containing protein kinase, for example its effect on the protein kinase activity. The compound may be tested in a screening method of the invention or other screening method. The compound may be formulated for pharmaceutical use, for example for use in *in vivo* trials in animals or humans, or for use in agriculture, for example as an antifungal agent.

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It may be useful to analyse a protein kinase structure (for example a structure determined or predicted for a complex of the protein kinase with a binding partner) in order to determine the activation state of the structure. This may be useful in further modelling binding of the binding partner to the protein kinase in other activation states, and in predicting how the binding partner may affect the activation state of the protein kinase or compete with other potential binding partners. It may also be useful in designing and assessing derivatives of the binding partner.

Thus, a further aspect of the invention provides a method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates. The method may further comprise the step of classifying the activation state of the structure as "open", "closed" or "intermediate". Details of the analysis, which involves the generation of eigenvectors and associated eigenvalues are given in Example 1. The analysis makes use of techniques described in Amadei et al (1993) Essential dynamics of proteins. Proteins 17, 412-425.

The hydrophobic/phosphate pocket-containing protein kinase may be PDK1. Alternatively, it may be an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2. Hydrophobic/phosphate pocket-containing protein kinases and their EMBL database accession numbers are listed in Table I. Sequences considered to form the phosphate binding pocket from representative hydrophobic/phosphate pocket-containing protein kinases are shown in Figure 5. All AGC family protein kinases other than PKA may be hydrophobic/phosphate pocket-containing protein kinases, as defined above. In addition to the protein kinases shown in Figure 7, rhodopsin and G-protein coupled receptor protein kinases, for example, may possibly also have a hydrophobic/phosphate pocket as defined above.

The terms SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, for example, as used herein include a polypeptide (a SGK, PKB, PKA, p70S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 polypeptide) comprising the amino acid sequence identified as a SGK, PKB, p70 S6

kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2, respectively, in the relevant EMBL database records indicated in Table 2.

Table 2

	Activation or T-	AGC	Accession
	Loop	Hydrophobic	number
•		Motif	
consensus:	$\underline{\mathtt{T}}\mathtt{FCGTxxYxAPD}$	FxxFSY	
	L E	$Y\underline{T}F$	
PKBα	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FPQF <u>S</u> Y	(Y15056)
РКВβ	$\underline{\mathtt{T}}$ FCGTPEYLAPE	FPQF <u>S</u> Y	(P31751)
$PKB\gamma$	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FPQF <u>S</u> Y	(AF135794)
SGK1	TFCGTPEYLAPE	FLGF <u>S</u> Y	(AAD41091)
SGK2	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	FLGF <u>S</u> Y	(AF169034)
SGK3	$\underline{\mathtt{T}}\mathtt{FCGTPEYLAPE}$	$\mathtt{FLGF}\underline{\mathtt{S}}\mathtt{Y}$	(AF169035)
PKCα	<u>T</u> FCGTPDYIAPE	FEGF <u>S</u> Y	(4506067)
РКСβІ	<u>T</u> FCGTPDYIAPE	FAGF <u>S</u> Y	(4506069)
РКСВП	<u>T</u> FCGTPDYIAPE	FEGF <u>S</u> F	(P05127)
РКСү	$\underline{\mathtt{T}}\mathtt{FCGTPDYIAPE}$	$\mathtt{FGGF}\underline{\mathtt{T}}\mathtt{Y}$	(P05129)
РКСδ	TFCGTPDYIAPE	FAGF <u>S</u> F	(5453970)
PCKζ _.	$\underline{\mathtt{T}}$ FCGTPNYIAPE	FEGFEY	(4506079)
PKCι	$\underline{\mathtt{T}}\mathtt{FCGTPNYIAPE}$	FEGFEY	(4506071)
PRK1	TFCGTPEFLAPE	FLDFDF	(AAC50209)
PRK2	$\underline{\mathtt{T}}\mathtt{FCGTPEFLAPE}$	FRDFDŸ	(AAC50208)
p70-S6 $K\alpha$	$\underline{\mathtt{T}}\mathtt{FCGTIEYMAPE}$	$\mathtt{FLGF}\underline{\mathtt{T}}\mathtt{Y}$	(AAA36410)
p70-S6Kβ	$\underline{\mathtt{T}}\mathtt{FCGTIEYMAPE}$	FLGFTY	(4506739)
p90-RSK1	<u>S</u> FCGTVEYMAPE	FRGF <u>S</u> F	(I38556)
p90-RSK2	<u>S</u> FCGTVEYMAPE	FRDF <u>S</u> F	(P51812)
p90-RSK3	<u>S</u> FCGTIEYMAPE	FRGF <u>S</u> F	(CAA59427)

MSK1	SFCGTIEYMAPD	FQGY <u>S</u> F	(AAC31171)
MSK2	<u>S</u> FCGTIEYMAPE	FQGYSF	(AAC67395)
PDK1	<u>S</u> FVGTAQYVSPE	(1)	(AF017995)

Table 2. Alignment of the amino acid sequences surrounding the T-loop and the hydrophobic motif of AGC kinases. All the sequences and accession numbers are from human proteins. The underlined residues correspond to those that become phosphorylated. Footnotes: (1) PDK1 does not possess a hydrophobic motif.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor et al (1999) Curr Biol 9, 186-197.

The PDK1 may also be a polypeptide with the amino acid sequence of residues 51 to 359 or 404 (or 71 to 360) of full-length human PDK1; this may comprise the protein kinase domain of PDK1, as described in Example 2. The PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may also be Myc epitope-tagged or His-tagged, as described in Example 1. The p70 S6 kinase, for example, may have a His tag at its N-terminus and/or may lack the carboxy terminal 104 residues (p70 S6K-T2). The PDK1 or SGK may

be a Saccharomyces cerevisiae homologue, for example Pkh1 or Pkh2 (PDK1 homologues) or Ypk1 or Yrk2 (SGK homologues), as described in Casamayor et al (1999) Curr Biol 9, 186-197.

It is particularly preferred, although not essential, that the variant or 5 fragment or derivative or fusion of the PDK1, or the fusion of the variant or fragment or derivative has at least 30% of the enzyme activity of full-length human PDK1 with respect to the phosphorylation of full-length human PKBa on residue Thr308 or SGK1 on residue Thr 256 in either the presence or absence of PtdIns(3,4,5)P₃ or PtdIns(3,4)P₂. It is more preferred if the 10 variant or fragment or derivative or fusion of the said protein kinase, or the fusion of the variant or fragment or derivative has at least 50%, preferably at least 70% and more preferably at least 90% of the enzyme activity of PDK1 with respect to the phosphorylation of PKBa or SGK1. However, it will be appreciated that variants or fusions or derivatives or fragments 15 which are devoid of enzymatic activity may nevertheless be useful, for example by interacting with another polypeptide. Thus, variants or fusions or derivatives or fragments which are devoid of enzymatic activity may be useful in a binding assay, which may be used, for example, in a method of the invention in which modulation of an interaction of a mutated PDK1 of the invention and optionally also PDK1 with a interacting polypeptide or compound, for example an interacting polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr, for example Phe/Tyr-Xaa-Xaa-Phe/Tyr-Asp/Glu-Phe/Tyr or Phe/Tyr-Xaa-Xaa-Phe/Tyr-PhosphoSer/PhosphoThr-Phe/Tyr is measured.

It is preferred that the variant or fragment or derivative or fusion of the said hydrophobic/phosphate binding pocket-containing protein kinase, or the fusion of the variant or fragment or derivative comprises a hydrophobic

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pocket and a phosphate binding pocket in the position equivalent to the hydrophobic and phosphate binding pocket of human PDK1, as discussed further below.

5 Equivalent preferences apply to a variant or fragment or derivative or fusion of the SGK, PKB, p70 S6 kinase, p90 RSK, PKCα, PKCδ, PKCζ or PRK2 (for example), or the fusion of the variant or fragment or derivative, with the substitution in relation to SGK, PKB and p70S6 kinase of the peptide substrate Crosstide (GRPRTSSFAEG), or for PKB and SGK of the peptide substrate RPRAATF; the substitution in relation to PKA of the peptide substrate Kemptide (LRRASLG); the substitution in relation to PKC isoforms and PRK1/2 of histone H1; and the substitution in relation to MSK1/2 or p90-RSK1/2/3 of CREBtide (EILSRRPSYRK).

15 By "variants" of a polypeptide we include insertions, deletions and substitutions, either conservative or non-conservative. In particular we include variants of the polypeptide where such changes do not substantially alter the activity of the said polypeptide, for example the protein kinase activity of PDK1, as described above.

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By "conservative substitutions" is intended combinations such as Gly, Ala; Val, Ile, Leu; Asp, Glu; Asn, Gln; Ser, Thr; Lys, Arg; and Phe, Tyr.

The three-letter amino acid code of the IUPAC-IUB Biochemical Nomenclature Commission is used herein, with the exception of the symbol Zaa (negatively charged amino acid). In particular, Xaa represents any amino acid. It is preferred that Xaa and Zaa represent a naturally occuring amino acid. It is preferred that at least the amino acids corresponding to the consensus sequences defined above are L-amino acids.

It is particularly preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of PDK1 referred to above (or the sequence for SGK (including SGK1, 2 and 3), PKB, PKA or p70 S6 kinase, for example, as appropriate, referred to above), more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 85%, in still further preference at least 80% in further preferably at least 95% or 97% identity with the amino acid sequence defined above.

It is still further preferred if the PDK1 (or SGK, PKB, PKA or p70 S6 kinase or other hydrophobic/phosphate binding pocket-containing kinase, as defined above) variant has an amino acid sequence which has at least 65% identity with the amino acid sequence of the catalytic domain, particularly the residues forming the hydrophobic pocket, of PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) in the appropriate sequence referred to above, more preferably at least 70%, 71%, 72%, 73% or 74%, still more preferably at least 75%, yet still more preferably at least 80%, in further preference at least 83 or 85%, in still further preference at least 90% and most preferably at least 95% or 97% identity with the amino acid sequence defined above. It will be appreciated that the catalytic domain of a protein kinase-related polypeptide may be readily identified by a person skilled in the art, for example using sequence comparisons as described below.

The percent sequence identity between two polypeptides may be determined using suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group and it will be appreciated that percent identity is calculated in relation to polypeptides whose sequence has been aligned optimally.

The alignment may alternatively be carried out using the Clustal W program (Thompson *et al* (1994) *Nucl Acid Res* 22, 4673-4680). The parameters used may be as follows:

Fast pairwise alignment parameters: K-tuple(word) size; 1, window size; 5, gap penalty; 3, number of top diagonals; 5. Scoring method: x percent.

Multiple alignment parameters: gap open penalty; 10, gap extension penalty; 0.05.

Scoring matrix: BLOSUM.

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It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide which consists of the amino acid sequence of the protein kinase PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase as the case may be) sequence referred to above or naturally occurring allelic variants thereof. It is preferred that the naturally occurring allelic variants are mammalian, preferably human, but may alternatively be homologues from parasitic or pathogenic or potentially pathogenic organisms. Examples of such organisms and homologues, and of uses of modulators of such homologues are given in US patent application No 60/112,114, filed on 14 December 1998, and applications claiming priority therefrom, or in Casamayor *et al* (1999) *Curr Biol* 9, 186-197.

It is preferred that the PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) is a polypeptide that is capable of interacting with a polypeptide comprising the amino acid sequence motif Phe/Tyr-Xaa-Xaa-Phe/Tyr, preferably Phe-Xaa-Xaa-Phe/Tyr, more preferably Phe-Xaa-Xaa-Phe, still more preferably Phe/Tyr-Xaa-Xaa-Phe/Tyr-Zaa-Phe/Tyr or Phe/Tyr-Xaa-Xaa-Phe/Tyr-COOH, for example the polypeptide PIF or PIFtide, as defined below. Further preferences for the said polypeptide are as given above.

The protein kinase activity of PKB, SGK or p70 S6 kinase that is modulated may be phosphorylation of the underlined residue in a polypeptide with the amino acid sequence Arg-Xaa-Arg-Xaa-Xaa-Ser/Thr. The polypeptide may be Glycogen Synthase Kinase 3 (GSK3), 40 S ribosomal subunit S6, BAD, 6-phosphofructo-2-kinase, phosphodiesterase3b, human caspase 9, endothelial nitric oxide synthase or BRCA1.

A compound identified by a method of the invention may modulate the ability of the protein kinase to phosphorylate different substrates, for example different naturally occurring polypeptides, to different extents. The compound may inhibit the protein kinase activity in relation to one substrate but may increase the protein kinase activity in relation to a second substrate. For example, the protein kinase activity of PDK1 may be modulated to a different extent for PKB when compared with SGK, p70 S6 kinase and/or PKC.

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It will be appreciated that the modulatory, for example inhibitory action of a compound found to bind (or inhibit binding of a polypeptide or compound) to the protein kinase may be confirmed by performing an assay of enzymic activity (for example PDK1 and/or PDK2 protein kinase activity) in the presence of the compound.

By "hydrophobic pocket-containing protein kinase having a hydrophobic pocket (PIF binding pocket) in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150," is meant a polypeptide

having an amino acid sequence identifiable as that of a protein kinase catalytic domain, and further having a predicted or determined three-dimensional structure that includes a hydrophobic pocket corresponding to the region indicated in Example 1 as the PIF binding pocket, and a pocket corresponding to the region indicated in Example 1 as the phosphate binding pocket. The hydrophobic pocket and phosphate binding pockets in PDK1 do not overlap with the ATP or phosphorylation site binding sites on PDK1.

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It is preferred that the protein kinase has identical or conserved residues that are equivalent to Lys 115, Ile118, Ile119, Val124, Val127 and/or Leu 155 of human PDK1, more preferably at least Lys115 and Leu155 of human PDK1, most preferably an identical residue equivalent to Leu155. Thus, for example, the protein kinase may have a Lys residue at the position equivalent to Lys115 of PDK1 and/or a Leu residue at the position equivalent to Leu155 of PDK1. It is preferred that the protein kinase does not have an Ala at the position equivalent to Lys115 and/or a Ser, Asp or Glu at the position equivalent to Leu155 of PDK1.

It is further preferred that the protein kinase has identical or conserved residues that are equivalent to Lys76, Arg131, Thr148 and/or Gln 150 of human PDK1, more preferably at least Lys76 and Gln150 of human PDK1, most preferably an identical residue equivalent to Gln150. Figure 5B shows an alignment of examples of protein kinases considered to have a phosphate binding pocket at the position equivalent to the said phosphate binding pocket of PDK1. Sequence conservation/preferred residues at the positions identified are discussed further in Example 1.

An amino acid sequence may be identifiable as that of a protein kinase catalytic domain by reference to sequence identity or similarities of three

dimensional structure with known protein kinase domains, as known to those skilled in the art.

Protein kinases show a conserved catalytic core, as reviewed in Johnson et al (1996) Cell, 85, 149-158 and Taylor & Radzio-Andzelm (1994) Structure 2, 345-355. This core folds into a small N-terminal lobe largely comprising anti-parallel β -sheet, and a large C-terminal lobe which is mostly α -helical. A deep cleft at the interface between these lobes is the site of ATP binding, with the phosphate groups near the opening of the cleft.

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Protein kinases also show conserved sequences within this catalytic core, and the residue equivalent to a given residue of, for example, PDK1, may be identified by alignment of the sequence of the kinase with that of known kinases in such a way as to maximise the match between the sequences. The alignment may be carried out by visual inspection and/or by the use of suitable computer programs, for example the GAP program of the University of Wisconsin Genetic Computing Group, which will also allow the percent identity of the polypeptides to be calculated. The Align program (Pearson (1994) in: Methods in Molecular Biology, Computer Analysis of Sequence Data, Part II (Griffin, AM and Griffin, HG eds) pp 365-389, Humana Press, Clifton).

The comparison of amino acid sequences or three dimension structure (for example from crystallography or computer modelling based on a known structure) may be carried out using methods well known to the skilled man, for example as described in WO 01/44497.

MAP kinase, MEK1, Cdk2 and Erk2 (for example) are not protein kinases having a hydrophobic pocket in the position equivalent to the hydrophobic (PIF binding) pocket of PDK1. MEK1, Cdk2 and ERK2 may have a larger

hydrophobic pocket which interacts with an amino acid sequence motif (which may be Phe-Xaa-Phe-Pro) which is not Phe-Xaa-Xaa-Phe. Thus, these protein kinases do not have a hydrophobic pocket in the position equivalent to the said hydrophobic (PIF-binding) pocket of PDK1.

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A further aspect of the invention provides a mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Vall27 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated. It is preferred that the said protein kinase is PDK1. The said protein kinase may alternatively be, for example, SGK, PKB or p70 S6 kinase. It is particularly preferred that the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala. The mutated protein kinase may be useful in determining whether a polypeptide or compound interacts with the hydrophobic (PIF binding) pocket or phosphate binding pocket of the unmutated protein kinase. For example, the abilities of a compound (including polypeptide) to bind to the mutated and unmutated protein kinase, or to modulate the activity of the protein kinase towards one or more substrates of the protein kinase, may be measured and compared.

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A further aspect of the invention provides a polynucleotide encoding a mutated protein kinase of the invention. A still further aspect of the invention provides a recombinant polynucleotide suitable for expressing a

mutated protein kinase of the invention. A yet further aspect of the invention provides a host cell comprising a polynucleotide of the invention.

A further aspect of the invention provides a method of making a mutated protein kinase of the invention, the method comprising culturing a host cell of the invention which expresses said mutated protein kinase and isolating said mutated protein kinase.

A further aspect of the invention provides a mutated protein kinase obtainable by the above method.

Examples of these aspects of the invention are provided in Example 1, and may be prepared using routine methods by those skilled in the art, for example as described in WO 00/35946.

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For example, the above mutated protein kinase may be made by methods well known in the art and as described below and in Example 1 or 2, for example using molecular biology methods or automated chemical peptide synthesis methods.

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It will be appreciated that peptidomimetic compounds may also be useful. Thus, by "polypeptide" or "peptide" we include not only molecules in which amino acid residues are joined by peptide (-CO-NH-) linkages but also molecules in which the peptide bond is reversed. Such retro-inverso peptidomimetics may be made using methods known in the art, for example such as those described in Mézière et al (1997) J. Immunol. 159, 3230-3237, incorporated herein by reference. This approach involves making pseudopeptides containing changes involving the backbone, and not the orientation of side chains. Retro-inverse peptides, which contain NH-CO

bonds instead of CO-NH peptide bonds, are much more resistant to proteolysis.

Similarly, the peptide bond may be dispensed with altogether provided that an appropriate linker moiety which retains the spacing between the $C\alpha$ atoms of the amino acid residues is used; it is particularly preferred if the linker moiety has substantially the same charge distribution and substantially the same planarity as a peptide bond.

It will be appreciated that the peptide may conveniently be blocked at its Nor C-terminus so as to help reduce susceptibility to exoproteolytic digestion.

The invention further provides a method of identifying a compound that modulates the protein kinase activity of a protein kinase having a hydrophobic pocket and phosphate binding pocket in the positions equivalent to the hydrophobic (PIF binding) pocket and phosphate binding pocket of PDK1, as defined above (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to the said mutated protein kinase of the invention.

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The method may further comprise determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated at the said residue. When the protein kinase is PDK1, it may lack a functional PH domain (ie it may lack a PH domain capable of binding a phosphoinositide).

It will be appreciated that the protein kinase or mutated protein kinase may be a fusion protein comprising a tag, for example to aid purification, for example a GST tag, as described in Example 1. The capability of the said PDK1 (or, for example, SGK, PKB, PKA or p70 S6 kinase) polypeptide with regard to interacting with or binding to a polypeptide or other compound may be measured by any method of detecting/measuring a protein/protein interaction or other compound/protein interaction, as discussed further below. Suitable methods include methods analagous to those described in Example 1, as well as other methods, for example yeast two-hybrid interactions, co-purification, ELISA, co-immunoprecipitation and surface plasmon resonance methods. Thus, the said PDK1 (or SGK, PKB, PKA or p70 S6 kinase) may be considered capable of binding to or interacting with a polypeptide or other compound if an interaction may be detected between the said PDK1 polypeptide and the said interacting polypeptide by ELISA, co-immunoprecipitation or surface plasmon resonance methods or by a yeast two-hybrid interaction or copurification method, for example as described in Example 1.

It is preferred that the interaction can be detected using a surface plasmon resonance method, as described in Example 1. The interacting polypeptide (for example a polypeptide comprising a phosphorylated "hydrophobic motif", for example S6K-pHM; see example 1) may be immobilised on the test surface, for example it can be coupled through amino groups to a SensorChip CM5TM, according to the manufacturer's instructions, or a biotinylated polypeptide can be bound to an avidin coated SensorChip SA. The protein kinase (at concentrations between, for example 0 and between 10μM and 1.0μM, for example 2μM) is then injected over the surface and steady state binding determined in each case. From these measurements a K_d can be determined. It is preferred that the interaction has a K_d of less than 8μM, more preferably less than 5μM, 2μM, 1μM, 500nM, 300nM, 200nM or 100nM, for example about 150nM. Alternatively, a K_d can be determined for a polypeptide or other compound in competition with the immobilised polypeptide (or other compound). The protein kinase (for

example at a concentration of 0.5 µM) is mixed with free polypeptide (for example, at concentrations between 0 and 3 µM) and the mixture injected over the immobilised polypeptides. The steady state binding is determined in each case, from which the K_d of the interaction can be determined using the Cheng-Prescott relationship. Alternatively, the interaction may be expressed in terms of an observed response or relative observed responses, measured in terms of mass of protein bound to the surface, as described in Example 2. For example, the polypeptide may be immobilised by amino coupling to a SensorChip CM5 and each protein kinase (for example different mutated protein kinases, as discussed below) for example at a concentration of 1.0 µM or a range of concentrations, injected over the immobilised polypeptide. Alternatively, the polypeptide may be immobilised on a SA SensorChip and each protein kinase, for example at a concentration of 40nM or a range of concentrations injected over the immobilised polypeptide. The steady state response for each protein kinase is determined, for example expressed in Response Units (RU). 1000RU corresponds to 1 ng/mm² of protein bound to the surface. A response of less than 10RU may indicate that no interaction has taken place. A response of at least 10RU may indicate that the immobilised and injected molecules interact with each other.

It will be appreciated that the above methods may be used to determine whether a particular polypeptide or compound interacts with a protein kinase or mutated protein kinase.

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The effect of the compound on the rate or degree of phosphorylation of a hydrophobic pocket and/or phosphate binding pocket-dependent substrate may be determined. A compound may be selected that decreases the protein kinase activity of the said protein kinase, for example PDK1, towards a hydrophobic pocket-dependent substrate or a phosphate binding

pocket-dependent substrate and does not affect or increases the protein kinase activity towards a hydrophobic pocket or phosphate binding pocket-independent substrate, for example PKB when the kinase is PDK1. An activator of PDK1 may mimic insulin and may be useful in treating diabetes or obesity, and may protect cells from apoptosis.

Compounds that bind specifically to the phosphate binding site may activate PDK1 (or other AGK kinase having a phosphate binding site). Also compounds that bind to the residues forming part of the pohsphate binding site might transduce the negative effect and inhibit the kinase activity. A compound interacting with the phosphate binding site of PDK1 may be an activator, but only of a subset of substrates. Some substrates of PDK1 require the interaction with the phosphate binding site, such as S6K and SGK.

To generate a specific molecule that could bind to the phosphate and/or PIF-binding pocket of PDK1 a anti-idiotype strategy using combinatorial RNA libraries could be employed. Previous studies have established that Combinatorial RNA libraries can be used to isolate specific ligands, called aptamers, for virtually any target molecule by a procedure probably best known as SELEX (Ellington, A. D., and Szostak, J. W. (1990) Nature 346, 818-822; Tuerk, C., and Gold, L. (1990) Science 249, 505-510). Using this approach RNA molecules that interact with antibodies raised against PIFtide or peptides that encompass the hydrophobic motif of AGC kinases which are phosphorylated at their hydrophobic motif would be selected (preferably antibodies that are specific for the phosphorylated form ie bind the phosphorylated form but not the non-phosphorylated form). These RNA species then may have the intrinsic conformation to interact with the phosphate binding (and possibly also the PIF-binding) pocket(s) of PDK1.

Antibodies to the phosphate binding pocket may be produced. For example, animals could be immunised with wild type PDK1. Serum could then be purified with a column where the resin is coated with wild type PDK1 used for the immunisation. Specific antibodies could then be passed through columns coated with mutant PDK1 molecules differing only in that they have specific mutations in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala. Antibodies that don't bind to this mutant will either be specific antibodies that recognise the specific motifs or antibodies that are sensitive to the conformational changes associated with these mutations. The opposite development could also be performed: antibodies against a mutant PDK1 having a specific mutation(s) in the phosphate binding pocket, such as Arg131, Lys76 or Gln150, for example mutated to Ala, could be produced and the serum further purified through columns coated with wild type PDK1.

Thus, a further aspect of the invention provides an antibody reactive with the phosphate binding pocket of PDK1 or other hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150. A further aspect of the invention provides an antibody reactive with PDK1 or other phosphate-binding pocket—containing protein kinase as defined above but not with the said protein kinase mutated at the phosphate binding site, or vice versa. A further aspect of the invention provides a method for preparing or selecting an antibody wherein the antibody is prepared or selected against a said protein kinase (for example

PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.

By the term "antibody" is included synthetic antibodies and fragments and variants (for example as discussed above) of whole antibodies which retain the antigen binding site. The antibody may be a monoclonal antibody, but may also be a polyclonal antibody preparation, a part or parts thereof (for example an F_{ab} fragment or F(ab')₂) or a synthetic antibody or part thereof. Fab, Fv, ScFv and dAb antibody fragments can all be expressed in and secreted from *E. coli*, thus allowing the facile production of large amounts of the said fragments. By "ScFv molecules" is meant molecules wherein the V_H and V_L partner domains are linked via a flexible oligopeptide. IgG class antibodies are preferred.

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Suitable monoclonal antibodies to selected antigens may be prepared by known techniques, for example those disclosed in "Monoclonal Antibodies: A manual of techniques", H. Zola (CRC Press, 1988) and in "Monoclonal Hybridoma Antibodies: techniques and Applications", JGR Hurrell (CRC Press, 1982), modified as indicated above. Bispecific antibodies may be prepared by cell fusion, by reassociation of monovalent fragments or by chemical cross-linking of whole antibodies. Methods for preparing bispecific antibodies are disclosed in Corvalen et al, (1987) Cancer Immunol. Immunother. 24, 127-132 and 133-137 and 138-143.

A general review of the techniques involved in the synthesis of antibody fragments which retain their specific binding sites is to be found in Winter & Milstein (1991) *Nature* 349, 293-299.

For example, an antibody that does not bind PDK1 Arg131Ala could be specifically recognising this residue in the phosphate binding site, but could

also be recognising specifically the inactive conformation of PDK1, which is stabilised by Arg 131. The opposite development could also be performed: antibodies against a mutant PDK1 Arg131Ala could be produced and the serum further purified through columns coated with wild type PDK1. In this way, antibodies may be prepared that would either not be able to interact with the phosphate binding site Arg 131 but only when a small residue is in its place, or antibodies that are probes for the active conformation of PDK1. These conformational probes could be used in high throughoutput screenings, HTS, in the search of compounds that are capable of modifying the conformation of the given protein kinase. Antibodies could have been produced with previous knowledge to detect active protein kinases by immunising with active protein kinases, but in those cases, the antibodies would have recognised also the phosphorylation events that make a protein kinase be active. In the methodology here described using the conformational probes could be easily isolated. antibodies, Furthermore, antibodies obtained from an active protein kinase (with overall modifications that make it active) could be further purified through a column coated with the inactive protein kinase (keeping the non bound fraction) and then further purifyied on a column coated with a protein kinase consisting of an activating mutation (such as R131A in the case of PDK1), retaining the specifically bound fraction, which could be an active conformation probe. This type of approach could also allow the development of conformation specific probes by the use of activating or inhibiting mutations.

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A further aspect of the invention provides a kit of parts useful in carrying out a method according to the preceding aspect of the invention, comprising (1) a mutated protein kinase of the invention and (2) the protein kinase which is not a mutated said protein kinase as defined above.

The protein structures described herein (for example with the co-ordinates shown in Examples 2, 3 or 4, or structures modelled thereon) may be useful in designing further reagents that may be useful in drug screening assays or characterisation of protein kinase activity or regulation. For example, such structures may be useful in designing mutants that may be useful in FRETbased activities, for example in which surface residues near to binding sites are mutated to cysteines to allow coupling of chromophores. For example, the cysteine residue may be fluorescently-labelled, and a change in fluorescence intensity or frequency may be detected in an assay. Any thiolreactive fluorophore, for example BADAN (see, for example, Wadum et al Fluorescently labeled bovine acyl-CoA binding protein - an acyl-CoA sensor. Interaction with CoA and acyl-CoA esters and its use in measuring free acyl CoA esters and non-esterified fatty acids (NEFA); Hammarstrom et al (2001) Biophys J 80(6), 2867-2885; Schindel et al (2001) Eur J Biochem 268(3), 800-808), could be used to label the cysteine. An alternative suitable fluorophore is Acrylodan (Richieri et al (1992) J Biol Chem 267(33), 23495-23501).

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20 It will be appreciated that the invention provides screening assays for drugs which may be useful in modulating, for example either enhancing or inhibiting, the protein kinase activity of a protein kinase (for example, the protein kinase activity towards a particular substrate) having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of Protein Kinase A (PKA) that is defined by residues including Lys76, Leu116, Val80 and/or Lys111 of full-length mouse PKA, for example PDK1, SGK, PKB, PKA or p70 S6 kinase, for example the PDK1 or PDK2 activity (as discussed above) of PDK1. The compounds identified in the methods may

themselves be useful as a drug or they may represent lead compounds for the design and synthesis of more efficacious compounds.

The compound may be a drug-like compound or lead compound for the development of a drug-like compound for each of the above methods of identifying a compound. It will be appreciated that the said methods may be useful as screening assays in the development of pharmaceutical compounds or drugs, as well known to those skilled in the art.

The term "drug-like compound" is well known to those skilled in the art, and may include the meaning of a compound that has characteristics that may make it suitable for use in medicine, for example as the active ingredient in a medicament. Thus, for example, a drug-like compound may be a molecule that may be synthesised by the techniques of organic chemistry, less preferably by techniques of molecular biology or biochemistry, and is preferably a small molecule, which may be of less than 5000 daltons. A drug-like compound may additionally exhibit features of selective interaction with a particular protein or proteins and be bioavailable and/or able to penetrate cellular membranes, but it will be appreciated that these features are not essential.

The term "lead compound" is similarly well known to those skilled in the art, and may include the meaning that the compound, whilst not itself suitable for use as a drug (for example because it is only weakly potent against its intended target, non-selective in its action, unstable, difficult to synthesise or has poor bioavailability) may provide a starting-point for the design of other compounds that may have more desirable characteristics.

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It is appreciated that screening assays which are capable of high throughput operation are particularly preferred. Examples may include cell based

assays and protein-protein binding assays. An SPA-based (Scintillation Proximity Assay; Amersham International) system may be used. For example, beads comprising scintillant and a substrate polypeptide or interacting polypeptide may be prepared. The beads may be mixed with a sample comprising ³²P- or ³³P-γ-labelled PDK1 or other protein kinase or mutated protein kinase (as defined above) and with the test compound. Conveniently this is done in a 96-well or 384-well format. The plate is then counted using a suitable scintillation counter, using known parameters for ³²P or ³³P SPA assays. Only ³²P or ³³P that is in proximity to the scintillant, i.e. only that bound to the substrate or interacting polypeptide that is bound to the beads, is detected. Variants of such an assay, for example in which the substrate or interacting polypeptide is immobilised on the scintillant beads *via* binding to an antibody or antibody fragment, may also be used.

It will be understood that it will be desirable to identify compounds that may modulate the activity of the protein kinase in vivo. Thus it will be understood that reagents and conditions used in the method may be chosen such that the interactions between, for example, the said protein kinase and the interacting polypeptide, are substantially the same as between the human protein kinase and a naturally occurring interacting polypeptide comprising the said amino acid sequence. It will be appreciated that the compound may bind to the protein kinase, or may bind to the interacting polypeptide.

The compounds that are tested in the screening methods of the assay or in other assays in which the ability of a compound to modulate the protein kinase activity of a protein kinase, for example a hydrophobic pocket-containing protein kinase, as defined above, may be measured, may be compounds that have been selected and/or designed (including modified)

using molecular modelling techniques, for example using computer techniques.

A further aspect of the invention is a compound identified or identifiable by the above selection/design methods of the invention, for example an RNA molecule or antibody identifiable as defined above.

A still further aspect of the invention is a compound (or polypeptide or polynucleotide) of the invention or identified or identifiable by the above selection/design methods of the invention, for use in medicine. Conditions or diseases in which such compounds, polypeptides or polynucleotides may be useful are indicated below.

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The compound (or polypeptide or polynucleotide) may be administered in any suitable way, usually parenterally, for example intravenously, intraperitoneally or intravesically, in standard sterile, non-pyrogenic formulations of diluents and carriers. The compound (or polypeptide or polynucleotide) may also be administered topically, which may be of particular benefit for treatment of surface wounds. The compound (or polypeptide or polynucleotide) may also be administered in a localised manner, for example by injection. The compound may be useful as an antifungal (or other parasitic, pathogenic or potentially parasitic or pathogenic organism) agent.

A further aspect of the invention is the use of a compound (or polypeptide or polynucleotide) as defined above in the manufacture of a medicament for the treatment of a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket, as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6

kinase/PRK2/PKC signalling. The patient may be in need of inhibition of a said hydrophobic/phosphate binding pocket-containing kinase in an infecting organism, for example the patient may have a fungal infection for which treatment is required. The compound may inhibit the infecting organism's (for example fungal) hydrophobic/phosphate binding pocket-containing protein kinase, but may not inhibit the patient's equivalent hydrophobic/phosphate binding pocket-containing protein kinase.

A further aspect of the invention is a method of treating a patient in need of modulation of signalling by a protein kinase having a hydrophobic/phosphate binding pocket as defined above, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound (or polypeptide or polynucleotide) as defined above.

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A compound that is capable of reducing the activity of PKC, for example PKCβ, PRK1 or 2, PDK1 (ie the PDK1 and/or the PDK2 activity), PKB, SGK or p70 S6 kinase may be useful in treating cancer. PDK1, for example via PKB and/or SGK, may be capable of providing a survival signal that protects cells from apoptosis induced in a variety of ways (reviewed in Cross et al (1995) Nature 378, 785-789 and Alessi & Cohen (1998) Curr. Opin. Genetics. Develop. 8, 55-62). Thus, such compounds may aid apoptosis. Reduction of the activity of PDK1, PKB, SGK and/or p70 S6 kinase may promote apoptosis and may therefore be useful in treating cancer. Conditions in which aiding apoptosis may be of benefit may also include resolution of inflammation.

A compound is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase may be useful in treating diabetes or obesity, or may be

useful in inhibiting apoptosis. Increased activity of PDK1, PKB, SGK or p70 S6 kinase may lead to increased levels of leptin, as discussed above, which may lead to weight loss; thus such compounds may lead to weight loss. For example, such compounds may suppress apoptosis, which may aid cell survival during or following cell damaging processes. It is believed that such compounds are useful in treating disease in which apoptosis is involved. Examples of such diseases include, but are not limited to, mechanical (including heat) tissue injury or ischaemic disease, for example stroke and myocardial infarction, neural injury and myocardial infarction. Thus the patient in need of modulation of the activity of PDK1, PKB, SGK or p70 S6 kinase may be a patient with cancer or with diabetes, or a patient in need of inhibition of apoptosis, for example a patient suffering from tissue injury or ischaemic injury, including stroke.

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- Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identified or identifiable by the screening methods of the invention.
- A still further invention provides a use of a compound identifiable by the screening methods of the invention in the manufacture of a medicament for treating an ischaemic disease in a patient.

Thus, a further aspect of the invention provides a method of treating a patient with an ischaemic disease the method comprising administering to the patient an effective amount of a compound identifiable by the screening methods of the invention.

If the patient is a patient in need of promotion of apoptosis, for example a patient with cancer, it is preferred that the compound of the invention that is

used in the preparation of the medicament is capable of reducing the activity of PDK1, PKB, SGK or p70 S6 kinase. If the patient is a patient with diabetes or a patient in need of inhibition of apoptosis, for example a patient with ischaemic disease, it is preferred that the compound of the invention that is used in the preparation of the medicament is capable of increasing the activity of PDK1, PKB, SGK or p70 S6 kinase.

All documents referred to herein are hereby incorporated by reference.

The invention is now described in more detail by reference to the following, non-limiting, Figures and Examples.

Figure legends

15 1. Overview of the PDK1 structure.

The PDK1 kinase domain backbone is shown in a ribbon representation, with the secondary structure elements for residues 74-163 in the lower half of the Figure and for residues 164- 358 in the upper part of the Figure. Helix αG , encompassing residues 287-295 (which makes a crystal contact to a symmetry related PDK1 molecule, Fig. 2), is at the bottom right of the Figure. Key residues discussed in the text are shown as a sticks model. ATP is shown as a sticks model. A simulated annealing $|Fo-|Fc\rangle$, ϕ calc map is shown in black, contoured at 3 σ . The phosphoserine and the sulphate discussed in the text are also shown.

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2. The PIF-pocket

A. A surface representation of the putative PIF binding pocket is shown and compared to the pocket interacting with the C-terminal FXXF motif in PKA. For PDK1, the αG helix of a symmetry-related molecule is shown as

a ribbon, in PKA the C-terminus is also shown as a ribbon. Aromatic amino acids buried in the pocket are shown as sticks; further side chains interacting with the pocket are also shown as sticks. Helix αC is also shown as a ribbon in both PDK1 and PKA (at bottom of images). In PDK1, the ordered sulphate ion and basic residues interacting with it are also shown.

B. A stereo image of the residues lining the PIF-pocket is shown. The PDK1 backbone is shown as a grey ribbon. Side chains are shown as sticks. Hydrogen bonds to the sulphate ion are shown as black dotted lines.

3. Structure-based sequence alignment

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The sequences of PKA and PDK1 are aligned according to a structural superposition performed in WHAT IF [Vriend, 1990]. Sequence numbering is according to PDK1. β -strands (arrows) and α -helices (bars) are shown for the PDK1 structure according to a DSSP [Kabsch and Sander, 1983] secondary structure assignment, and labelled consistent with the secondary structure element names proposed for PKA [Taylor and Radzioandzelm, 1994]. Residues lining the PIF-pocket are indicated with a black dot. Residues hydrogen bonding the sulphate ion are indicated by arrows. The PDK1 residues equivalent to Ser53 and Gly186 in PKA, are labelled with an asterisk.

4. PDK1 binding & activation studies

Binding and activation of wild type and mutant forms of PDK1 to a phosphopeptide derived from the hydrophobic motif of S6K1. The binding of the wild type (wt) PDK1 and indicated mutants to a phosphopeptide comprising the hydrophobic motif of S6K1 (S6K-pHM: SESANQVFLGFT*YVAPSV, where T* indicates phospho-threonine) was analysed by surface plasmon resonance as described in the Materials and Methods.

A. The sensor chip SA was coated with 12RUs of the biotinylated S6K-pHM peptide and the binding was analysed following injection of 270 nM wild type PDK1, PDK1 [T148A] and PDK1 [K76A]. No detectable binding to S6K-pHM was observed using PDK1 [R131A] or PDK1 [Q150] (data not shown).

B. As in **A.** except that binding was analysed over a range of PDK1 concentrations (2-2150nM). The response level at the steady state binding is plotted versus the log of the PDK1 concentration. The estimated Kd was obtained by fitting the data to a sigmoid curve using Kaleidagraph software.

10 Kd for wild type PDK1 was 642 - 131 nM, PDK1 [T148A] was 64 - 7 nM and PDK1 [K76A] was 1744 - 167 nM. No detectable binding of PDK1 to the non-phosphorylated S6K-HM peptide (SESANQVFLGFTYVAPSV) was detected with wild type PDK1 or any of the mutants (data not shown).

C. Activation of the indicated forms of PDK1 by S6K-pHM and S6K-HM. PDK1 activity was measured using the peptide substrate (T308tide) in the presence of the indicated concentrations of S6K-pHM (closed circles) and S6K-HM (open circles) as described in the methods. Assays were performed in triplicate and similar results obtained in 2 separate experiments. The results are the average – SD for a single experiment.

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5. Interactions of regulatory phosphates with the αC helix

A. The PDK1 backbone is shown as a ribbon, with helix α C in the centre of the view. Key residues are shown as sticks. The sulphate ion and the phosphate on the activation loop are also shown. A sticks model of ATP is shown. Hydrogen bonds are shown as black dotted lines.

B. Alignment of the amino acid sequence forming part of the phosphate pocket on PDK1 with the equivalent region of the indicated AGC kinases. Identical residues are denoted by white letters on a black background and similar residues by gray boxes. Arrows indicate the residues corresponding to Lys 76, Arg131, Thr148 and Gln150 of PDK1.

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6. Essential dynamics

- A. Projection of all available PKA crystal structures (labelled dots) and the PDK1 structure (diamond) onto the first two eigenvectors (i.e. the ones with the two largest eigenvalues) calculated from the PKA structures.
- B. Graphic representation of the motion along the first eigenvector, generated by projecting two structures at -4 nm (black) and +4 nm (grey).

7. Alignment of AGC protein kinase family members.

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Example 1: High resolution crystal structure of the human PDK1 catalytic domain defines the regulatory phosphopeptide docking site

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The 3-Phosphoinositide Dependent Protein Kinase-1 (PDK1) plays a key role in insulin/growth factor induced signalling pathways through phosphorylation of downstream AGC-kinases such as Protein Kinase B/Akt and p70 ribosomal S6 kinase (S6K1). Here we describe the 2.0 Å crystal structure of the PDK1 kinase domain in complex with ATP. The structure defines the hydrophobic pocket termed the 'PIF-pocket'which plays a key role in mediating the interaction and phosphorylation of certain substrates such as S6K1. In the PDK1 structure, this pocket is occupied by an extensive crystallographic contact with another molecule of PDK1, reminiscent of the interaction of Protein Kinase A with the hydrophobic motif at its C-terminus. Previous studies have shown that phosphorylation of S6K1 at its C-terminal PIF-pocket-interacting motif, promotes the binding of S6K1 with PDK1, suggesting that there may be a phosphate docking site located nearby the PIF-pocket. Interestingly, close to the PIF-pocket on the PDK1 structure, there is an ordered sulphate ion, interacting

tightly with four surrounding side chains. The roles of these residues were investigated through a combination of site directed mutagenesis and kinetic studies, the results of which suggest that this region of PDK1 does indeed represent a phosphate dependent docking site. An analogous phosphate binding regulatory motif may participate in the activation of other AGC kinases.

Results & Discussion

Overall structure

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The structure of the catalytic domain of PDK1 was solved by molecular replacement and refined to an R-factor of 0.19 (Rfree=0.22). PDK1 assumes the classic bilobal kinase fold (Fig. 1) and is similar to the only other AGC kinase structure solved, that of PKA (RMSD of 1.0 Å on C α atoms with PDB entry 1STC [Prade et al., 1997]). The form of PDK1 that was crystallized comprised residues 51 to 359. The tip of the activation loop (residues 233-236) is disordered, as observed in other kinase structures [Johnson et al., 1996]. The N-terminus (residue 51-70), which is pointing into a large void generated by the crystallographic symmetry, is also disordered. In contrast, the N-terminal extension to the kinase domain of PKA assumes an amphipathic a -helix (termed αA-helix), and packs against the kinase core [Knighton et al., 1991]. The cluster of hydrophobic residues that mediates this interaction in PKA is not present in PDK1, suggesting that the N-terminus of PDK1 could have a different function from that of PKA. Interestingly, it has recently been shown that the N-terminus of PDK1 (residues 1-50) interacts with Ral guanine nucleotide exchange factors [Tian et al., 2002]. Thus, this region may assume a unique conformation in PDK1, which is not defined by the structure described here.

PDK1 was crystallised in the presence of ATP but in the absence of any divalent cations. In the early stages of the refinement well-defined density for the entire ATP molecule could be observed. ATP adopts a different conformation to that observed in other kinase-ATP complexes (Fig. 1). Perhaps due to the absence of divalent cations, the generally observed kink between the β and γ phosphate caused by the interaction with such an ion, is not seen in the PDK1 structure.

It is known that PDK1 can phosphorylate itself on residue Ser 241 in the activation loop and that this phosphorylation is required for PDK1 activity [Alessi et al., 1997]. Indeed, we observed density for a phosphate attached to this residue (Fig. 1), and extensive interactions are observed between this phosphoserine and residues from the C-terminal lobe and α C-helix (Fig. 1). The interaction between Ser241 and the C-terminal lobe is similar to the equivalent interactions in PKA but as discussed below the binding to the α C-helix differs.

The PIF-pocket

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As outlined in the introduction, PDK1 was postulated to possess a pocket (the 'PIF-pocket') in the small lobe of its catalytic domain, required for the binding of PDK1 to the hydrophobic motif of its substrates [Biondi et al., 2000]. The PDK1 structure described here indeed reveals such a pocket, and shows that it lies in a location similar to the FXXF-binding pocket in PKA (Fig. 2). PDK1 residues Lys115, Ile118, Ile119 on the αB helix (Fig. 2), Val124, Val127 on the αC helix and Leu155 on β-sheet 5 form an approximately 5 Å deep pocket. Previous work has shown that mutation of Leu 155 to Glu abolishes the ability of PDK1 to interact with a peptide that encompasses the hydrophobic motif of PRK2 (PIFtide) [Biondi et al., 2000]

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as well as with S6K1, SGK1, PKC and PRK2 [Balendran et al., 2000, Biondi et al., 2000]. In addition, mutation of Lys115, Ile119, Glu150, and Leu155 to alanine, reduced the affinity of PDK1 for PIFtide approximately 10-fold, but did not affect the ability to phosphorylate and activate S6K1 and SGK1 [Biondi et al., 2001]. These results are in agreement with the crystal structure of the PIF-pocket, since Leu155 is located at the center and the other residues line the wall of the pocket (Fig. 2). Interestingly, in our structure, the PIF-pocket is occupied by helix αG of a symmetry related molecule (Fig. 2). Tyr288 and Phe291 make hydrophobic contacts in this pocket with almost all pocket-lining residues, remarkably reminiscent of the interactions of the phenylalanines in the FXXF motif in PKA and their hydrophobic docking site in the equivalent region of the kinase domain (Fig. 2). In addition, residues Glu287, Gln292, Ile295 and Lys296 on the symmetry related loop also form contacts with residues lining the PIFpocket. In total, 244 ² Å of accessible surface is buried by this contact, suggesting this is a tight interaction. However, the significance of this interaction is not clear as an oligomerisation event for PDK1 has not been demonstrated in solution previously. Indeed both the isolated catalytic domain of PDK1 that was crystallised and full length PDK1 migrate in gel filtration chromatography as apparent monomeric species (data not shown).

The phosphate pocket

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As outlined in the introduction, substrates of PDK1, such as S6K1, interact with the PIF-pocket of PDK1 with higher affinity when they are phosphorylated at their hydrophobic motif. This suggested that a regulatory phosphate binding site may be located close to the PIF-pocket. During refinement of the PDK1 structure, it became clear that next to the PIF-pocket another small pocket was present, occupied by a tetrahedral oxy-

anion (Fig. 2). As 2.0 M of sulphate was present in the crystallisation conditions, this was assigned as a sulphate ion. The ion interacts with four residues lining the pocket, namely Lys76, Arg131, Thr148 and Gln150. Because of its close proximity to the PIF-pocket (approximately 5Å) it is possible that this sulphate-occupied pocket could represent the binding site for the phosphate on the phosphopeptide. To investigate this further, we mutated Lys76, Arg131, Thr148 and Gln150 to Ala, in order to verify the contribution of each of these residues in enabling PDK1 to interact with a peptide encompassing the hydrophobic motif of S6K1, in which the residue equivalent to Thr412 was phosphorylated (termed S6K-pHM). A quantitative surface plasmon resonance based binding assay (Fig. 4A) showed that wild type PDK1 interacted with S6K-pHM, with a Kd of 0.6 μM with S6K-pHM but not detectably to the non-phosphorylated form of this peptide (S6K-HM). The PDK1[R131A] and PDK1[Q150A] mutants did not detectably interact with S6K-pHM in this assay (Fig. 4B), confirming that the interactions these residues make in the PDK1 structure are of key importance. The PDK1[K76A] mutant interacted with 3-fold lower affinity (Kd 1.7 μ M) with S6K-pHM. The PDK1[T148A] mutant however possessed about 10-fold higher (Kd 0.06 µM) affinity for S6KpHM than wild type PDK1. Moreover, the dissociation of PDK1[T148A] from S6K-pHM is markedly slower than that of wild type PDK1 or PDK1[K76A] (Fig 4A). These findings are unexpected as Thr148 is within hydrogen bonding distance of the sulphate (Fig. 2), but indicate that this residue may play a role in enabling the dissociation of PDK1 from S6KpHM.

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The binding of PDK1 to PIFtide stimulates up to 4-fold the rate at which PDK1 phosphorylates a small peptide that encompasses the activation loop motif of PKB (termed T308tide) [Biondi et al., 2000], indicating that occupancy of the PIF-pocket of PDK1 activates the enzyme. Similarly, the

binding of a phosphopeptide corresponding to the hydrophobic motif of RSK stimulated PDK1 activity 6-fold [Frodin et al., 2000]. We have now also found that the binding of S6K-pHM to wild type PDK1 induces a maximal 5-fold activation, with a half maximal activation occurring at a concentration of approximately 50 µM S6K-pHM (Fig. 4C). We next specific activities of PDK1[K76A], assayed the PDK1[R131A], PDK1[T148A] and PDK1[Q150A] mutants in the absence and presence of increasing concentrations of S6K-pHM (Fig. 4C). The PDK1[K76A] possessed the same specific activity towards T308tide in the absence of S6K-pHM as wild type PDK1, but an approximately 3-fold higher concentration of S6K-pHM was required to half maximally activate PDK1[K76A], consistent with the reduced affinity of this form of PDK1 for S6K-pHM (Fig. 4A,B). The PDK1[R131A] mutant possessed a 3-fold higher specific activity towards Thr308tide in the absence of S6K-pHM (Fig. 4C), as has been observed previously with certain other PIF-pocket mutants of PDK1(PDK1[K115A] and PDK1[L155E]) [Biondi et al., 2000]. However, in accordance with the inability of PDK1[R131A] to bind S6KpHM in the Biacore assay (Fig. 4B), it was not significantly activated by concentrations of S6K-pHM below 0.1 mM and its activity was only moderately further increased by the addition of high concentrations (0.3 and 1 mM) of S6K-pHM (Fig. 4C). The activity of a mutant of PDK1 in which both Lys76 and Arg131 were changed to Ala was activated even less significantly by these high concentrations of S6K-pHM. The PDK1[T148A] and PDK1[Q150A] mutants possessed similar specific activity towards T308tide as wild type PDK1 in the absence of S6K-pHM. The PDK1[T148A] mutant was activated similarly as wild type PDK1 by S6KpHM and consistent with the inability of PDK1[Q150A] to interact with S6K-pHM, this mutant of PDK1 was not significantly activated by concentrations of S6K-pHM below 0.1 mM but at 0.3 and 1 mM peptide a 2-3 fold activation was observed (Fig. 4).

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At very high peptide concentrations (0.3-1 mM) the non-phosphorylated S6K-HM peptide induced a small (<2-fold) activation of PDK1 (Fig. 4C). Interestingly, despite the PDK1[K76A] and PDK1[R131A] mutants being markedly less able to interact with the phosphorylated S6K-pHM peptide, than wild type PDK1, high concentrations of the S6K-HM peptide activated PDK1[K76A] and PDK1[R131A] to a similar extent as wild type PDK1, indicating that the ability of these mutants to interact weakly with the S6K-HM peptide was not affected.

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We evaluated the sequence conservation in the phosphate pocket of the insulin/growth factor-activated AGC family kinases (PKB α , S6K1, SGK1 and RSK1). Sequence alignments indicate that this pocket is conserved amongst these kinases (Fig 5A). The most conserved residue is Gln150 which is found in all of these AGC kinases and the residue equivalent to Lys76 is always a basic residue (Fig. 5A). Arg131 is conserved in S6K1, SGK1 and RSK1 but not in PKB α , or PKB β or PKB γ , where it is an Asn or Ser. Thr148 is conserved in PKB α and SGK1 but is an Ala in S6K1 and RSK1. Interestingly, we have found the Thr 148Ala mutation in PDK1 did not disrupt the phosphate pocket (Fig 4). As PKB α , S6K1, SGK1 and RSK1 require to be phosphorylated at their hydrophobic motif to be maximally activated, it is tempting to speculate that the C-terminal hydrophobic motifs of these enzymes, when phosphorylated, bind to their own PIF/phosphate pockets, thereby generating a network of interactions similar to that of PDK1. In support of this, PKB $\!\alpha$, S6K1, SGK1 and RSK1 also require phosphorylation of their activation loop at the position equivalent to Ser241 for activity. Consistent with PKA not possessing a phosphate pocket, Lys76 and Gln150 are not conserved in PKA (Fig. 3), and indeed such a pocket is not observed in the PKA structure (Fig. 2).

The αC helix

The PDK1 structure shows that, as in other protein kinases [Johnson et al., 2001, Husen and Kuriyan, 2002], the α C helix (residues 124-136) is a key signal integration motif in the kinase core. One turn of the PDK1 α C helix (residues 129-131, Figs. 3, 5) links together the N-terminal lobe, the C-terminal lobe and the active site. Arg129 points towards the activation loop and forms two hydrogen bonds with the phosphorylated Ser241, whereas Arg131 forms two hydrogen bonds with the sulphate in the phosphate pocket (Fig. 5). Glu130 coordinates Lys111 which forms a hydrogen bond with the α -phosphate of the bound ATP. This interaction is conserved in all protein kinases and shown to be crucial for activation [Johnson et al., 2001, Husen and Kuriyan, 2002]. An additional residue, His126, forms a third hydrogen bond with the phosphorylated Ser241. Val124 and Val127 on the α C helix are involved in formation of the PIF-pocket (Fig. 5).

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The αC helix provides a structural link between the putative phosphopeptide binding pocket and the phosphoserine in the activation loop. The fact that R131A has higher basal activity than wild type PDK1 may indicate that this residue plays tuning role in the PDK1 structure, not only participating in the activation of PDK1 in the presence of a phosphate ion, but also on keeping the equilibrium of the enzyme towards an inactive conformation in the absence of S6K-pHM. To our knowledge this is the first report of a kinase structure in which the αC helix is positioned by 2 regulatory phosphate binding sites on either side of the helix (Fig 5). This provides a possible sensor-mechanism for linking the phosphorylation-state of the activation loop and the phosphopeptide binding event in the PIF-pocket to PDK1 activity.

Activation state

All structures of PKA solved to date show a phosphorylated T-loop and are therefore assumed to be in an active state. In addition to the unphosphorylated versus phosphorylated states of PKA, there appear to be two main conformational states possible for the latter [Zheng et al., 1993, Johnson et al., 2001]. In the active, closed conformation, all residues are positioned to facilitate phosphoryl transfer. In contrast, the inactive, open conformation is seen in absence of a nucleotide, and differs from the closed conformation by conformational changes of the N-terminal and C-terminal domains with respect to each other. In addition, three 'intermediate' structures were described from PKA, having either adenosine (PDB entry 1BKX [Narayana et al., 1997]) or the inhibitors staurosporine (PDB entry 1STC [Prade et al., 1997]) and balanol (PDB entry 1BX6 [Narayana et al., 1999]) in the ATP-binding site. Taylor and colleagues have described a method to distinguish between the active and inactive conformations, based on three distances: His87-pThr197 (aC helix positioning), Ser53-Gly186 (opening of the glycine-rich loop) and Glu170-Tyr330 (C-terminal tail distance to active site) [Johnson et al., 2001]. In PDK1, only one of these distances, the opening state of the glycine rich loop, can be measured due to sequence conservation (Fig. 3). This distance is 12.4 Å, similar to a PKA intermediate conformation (this distance in PKA is 14.2Å for the open, 11.8 Å for intermediate and 10.0 Å for the closed conformation [Johnson et al., 2001]). To allow a more direct comparison of the PDK1 structure with the available PKA structures, we have analysed the conformational state of PDK1 in detail using a novel approach, which involves a principal component analysis (also called "essential dynamics" [Amadei et al.,1993]) of the crystallographic coordinates. In short, this involves the construction of a covariance matrix containing the correlations between atomic shifts (with respect to an average structure) in the ensemble of all available PKA crystal structures. Diagonalisation of this matrix gives eigenvector/eigenvalue sets which describe concerted shifts of atoms

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(eigenvectors) together with the corresponding mean square fluctuation of the structures (eigenvalues). This approach allows a condensed description of PKA conformational states using only a few degrees of freedom, as shown previously for a range of other proteins [van Aalten et al., 1997,van Aalten et al., 2000,deGroot et al., 1998]. Diagonalisation of a covariance matrix built from the backbone atoms of residues 37-196, 198-283 and 286-305 results in a set of eigenvectors that describe concerted motions of the PKA backbone. In Fig. 6A, all PKA structures are projected on a subspace spanned by the first two eigenvectors (i.e. those with the two largest eigenvalues). It appears that the PKA structures cluster in three main areas along the first eigenvector. On the left of the average structure (which by definition has a projection of 0.0 on all eigenvectors) are the structures that are known to be in the "open" conformation (Fig. 6A). Around the average structure lie the structures that have been shown to be in an "intermediate" conformation (complexes with the inhibitors staurosporine, balanol and adenosine). More to the right of the average structure are the PKA structures that are known to be in the "closed" conformation. Thus, we have captured the conformational state of PKA in a single variable, the translation along the first eigenvector. This is further clarified by investigation of the atomic shifts described by this eigenvector in Cartesian space (Fig. 6B). A hinge-bending motion is observed between the Nterminal and C-terminal lobes, opening and closing the active site. It is now possible directly to compare the PDK1 conformational state by projecting the structure (backbone atoms only) onto the PKA eigenvectors. Fig. 6A shows that the conformation of PDK1 is close to the PKA structures that are in an "intermediate" conformation, consistent with the other structural analyses described above.

Conclusions

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We have reported the structure of the PDK1 catalytic domain, which, although similar to PKA, has revealed important features that increase our understanding of the mechanism by which PDK1 is regulated. The structure, together with mutational analyses, defines a phosphopeptide binding pocket, consisting of a separate hydrophobic PIF-pocket and a phosphate binding site, which mediates the interaction of PDK1 with the phosphorylated hydrophobic motif of S6K. This is consistent with the previous hypothesis that phosphorylation of S6K and SGK [Biondi et al., 2001] as well as RSK [Frodin et al., 2000] at their FXXFS/T hydrophobic motif is the trigger for their interaction and phosphorylation by PDK1. In this mechanism the PIF-pocket would physiologically only interact with the Phe residues when the Ser/Thr residue is phosphorylated. Furthermore, as the phosphate pocket is conserved in other AGC kinases, the structural features and network of interaction of the phosphate pocket with the α Chelix on PDK1, could provide insight into the mode of activation of other AGC kinases.

Experimental Procedures

20 Materials

Mammalian and Insect cells culture reagents were from Life Technologies. SensorChips SA were from BiaCore AB. Glutathione Sepharose, as well as pre-packed HiTrap Q HP and Hiload Superdex 200 prep grade columns were from Amersham Biosciences. Dialysis cassettes were from the Slide-A-Lyzer series (Pierce). Ni-NTA Agarose was from Qiagen. Disposable ultrafiltration devices (polyethersulfone membranes) were from Vivascience. Crystallisation research tools (primary screens, additive

screens and crystallisation plates) were from Hampton Research. Peptides were synthesised by Dr G. Blomberg (University of Bristol, UK).

General methods

Molecular biology techniques were performed using standard protocols. Site directed mutagenesis was performed using a QuickChange kit (Stratagene) following instructions provided by the manufacturer. DNA constructs used for transfection were purified from bacteria using Qiagen plasmid Mega kit according to the manufacturer's protocol, and their sequence verified. Human kidney embryonic 293 cells were cultured on 10 cm diameter dishes in Dulbecco's modified Eagle's medium containing 10% foetal bovine serum.

Buffers

Low Salt Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl; High Salt Buffer: 25mM Tris-HCl pH 7.5, 500 mM NaCl. Lysis Buffer: 25mM Tris-HCl pH 7.5, 150 mM NaCl 0.07% β -mercaptoethanol, 1mM Benzamidine, and 20 μg/ml PMSF. Buffer A: 50 mM Tris-HCl pH 7.5, 1 mM EGTA, 1 mM EDTA, 1% (by mass) Triton-X 100, 1 mM sodium orthovanadate, 50 mM sodium fluoride, 5 mM sodium pyrophosphate, 0.27 M sucrose, 1 μM microcystin-LR, 0.1% (by vol) β -mercaptoethanol and "complete" proteinase inhibitor cocktail (one tablet per 50 ml, Roche). Buffer B: 50 mM Tris/HCl pH 7.5, 0.1 mM EGTA, 10 mM β -mercaptoethanol and 0.27 M sucrose.

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Expression, purification and characterisation of the kinase domain of PDK1

A cDNA encoding for human PDK1 amino acid residues 51-359 with a stop codon inserted at position 360, was amplified by PCR reaction using full length human PDK1 cDNA in the pCMV5 vector [Alessi et al., 1997] as a template a 5'primer, which incorporates a BamH1 restriction site, an initiating methionine, a hexahistidine tag.followed by a PreScission protease recognition sequence prior to the residue equivalent to Met51 of PDK1 (ggatcctataaatatggcacatcatcatcatcatctggaagttctgttccaggggcccatggacggcact gcagccgagcctcgg) and the 3' primer applied in this reaction was: 5'ggatcctcaggtgagcttcggaggcgtctgctggtg-3'. The resulting PCR product was ligated into pCR 2.1 TOPO vector (Invitrogen) and then subcloned as a BamH1-BamH1 fragment into pFastbac1 vector (Life Technologies) for baculovirus protein expression. The resulting construct was then used to generate recombinant baculovirus using the Bac-to-Bac system (Life Technologies) following the manufacturer's protocol. The resulting baculoviruses were used to infect Sf21 cells at 1.5 x 106/ml. The infected cells were harvested by centrifugation 72 hours post infection. Cell pellets corresponding to 7 l of culture were resuspended in 900 ml of Lysis Buffer and cells lysed in nitrogen cavitation chamber. Cell debris was then pelleted by centrifugation, the supernatant made 0.5 M NaCl by addition of 4M NaCl and then incubated with Ni-NTA-Agarose (10 ml resin) for one hour. The resin was then washed in 10 times with 40 ml of Lysis Buffer containing 0.5M NaCl and then placed in a disposable Econo-Pac column (BioRad), where the resin was further washed with 700 ml of high salt buffer and then with 100 ml of low salt buffer, both supplemented with 10 mM imidazole. Elution was performed with 200 mM imidazole in high salt buffer and 2 ml fractions were collected. Fractions containing protein were pooled, diluted to 200 mM NaCl with 25 mM Tris/HCl pH 7.5, and loaded onto a 5 ml Hi-trap Q sepharose column. The flow-through from this step, containing PDK1, was concentrated to 4 ml and then chromatographed on a 16/60 Superdex 200 gel filtration column using an AKTA Explorer system

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(Amersham Biosciences) equilibrated with high salt buffer with the addition of 1mM DTT. PDK1 eluted in a large symmetric peak at the expected size for a monomer. The PDK1 containing peak was again pooled, concentrated and incubated with 300 µg GST-PreScission protease (expression construct kindly provided by John Heath, University of Birmingham, UK) on ice for 4h. In order to eliminate the cleaved His-tag sequences as well as any remaining uncleaved His-PDK1 and the GST-PreScission protease, the mixture was incubated with a mixture of 200 µl glutathione-Sepharose and 200 µl Ni-NTA agarose resin for 15 minutes and the PDK1 protein that did not bind was collected. The resulting protein consists of PDK1 (51-359) preceded by a Gly-Pro at the N-terminus. The protein at this stage of the purification was apparently homogeneous as revealed by a single band after electrophoresis of 20 µg of protein on SDS-PAGE and staining with Coomasie Brilliant Blue R250 (data not shown).

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Electrospray mass spectrometry revealed a main peak mass close to the expected size of this fragment of PDK1. The specific activity of PDK1 (51-359) towards the peptide T308tide and its activation in the presence of PIFtide was identical to wild type full length PDK1 [Biondi et al., 2000], and tryptic peptide mass finger printing indicated that PDK1 was quantitatively phosphorylated at Ser241 (data not shown). In BiaCore experiments, the steady state binding of PDK1 (51-359) to the peptide PIFtide was similar to that of the His-tag PDK1 (51-556) protein characterised previously [Balendran et al., 1999a].

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Crystallisation and data collection

The PDK1 (51-359) protein was concentrated to a final concentration of 8.5 mg/ml (as determined by a Bradford assay using bovine serum albumin as a

standard). The sitting drop vapour diffusion method was used for producing crystals. Sitting drops were formed by mixing 1 µl of protein solution with 1 µl of a mother liquor solution (0.1 M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP) with the addition of 0.2 µl EDTA (100mM). Hexagonal crystals (Table I) of PDK1 were grown at 20° C from a mother liquor containing 0.1M Tris/HCl pH 8.5, 2.0 M ammonium sulphate, 16.6 mM ATP). Crystals appeared after one day, growing to 0.05 x 0.05 x 0.2 mm over 20 days. Crystals were frozen in a nitrogen gas stream after being soaked in 0.075 M Tris 8.5, 1.5M ammonium sulphate, 25% (v/v) glycerol.

Expression and purification of wild type and mutant forms of GST-PDK1.

Wild type-PDK1 [Alessi et al., 1997], PDK1[R76A], PDK1[R131A], PDK1[R76A,R131A], PDK1[T148A] and PDK1[Q150A] in the pEBG2T vector were used to express the wild type and indicated mutants of PDK1 fused through their N-terminus to glutathione S-transferase (GST). The GST fusion proteins were expressed in human embryonic kidney 293 cells. For the expression of each construct, twenty 10 cm diameter dishes of 293 cells were cultured and each dish transfected with 10 µg of the pEBG-2T construct, using a modified calcium phosphate method. 36 h post-transfection, the cells were lysed in 0.6 ml of ice-cold Buffer A, the lysates pooled, centrifuged at 4 ° C for 10 min at 13000 g and the GST-fusion proteins were purified by affinity chromatography on glutathione-Sepharose and eluted in Buffer B supplemented with 20 mM glutathione as described previously [Alessi et al., 1997]. Typically between 1 and 2mg of each GST-fusion protein was obtained and each protein was more than 75 judged by SDS polyacrylamide gel electrophoresis (data not shown).

PDK1 catalytic activity measurements

The ability of wild type and mutant PDK1 to phosphorylate the synthetic peptide T308tide (KTFCGTPEYLAPEVRR ([Biondi et al., 2000]) was carried out in 30 µl assays containing 100 ng of wild type or mutant PDK1, 50 mM Tris/HCl pH 7.5, 0.1% β -mercaptoethanol, 10 mM MgCl₂, 100 μ M [32y P]ATP (200 cpm/pmol), 0.5 µM microcystin-LR, 1 mM T308tide in the presence or absence of the indicated concentrations of the S6K-pHM (SESANQVFLGFT(P)YVAPSV) S6K-HM.peptide peptide or (SESANQVFLGFTYVAPSV). After incubation for 10 min at 30 $^{\circ}$ C, 25 μl of the resultant mixture was spotted into P81 phosphocellulose paper (2 x 2 cm) and the papers washed and analysed as described previously for assays of MAP kinase. Control assays were carried out in parallel in which either PDK1, or peptide substrate were omitted; these values were always less than 5% of the activity measured in the presence of these reagents. One Unit of PDK1 activity was defined as that amount required to catalyse the phosphorylation of 1 nmol of the T308tide in 1 min.

Biacore analysis

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Binding was analysed in a BiaCore 3000 system (BiaCore AB, Stevenage, UK). Biotinylated S6K-pHM (Biotin-C₁₂- SESANQVFLGFT(P)YVAPSV) or the non-phosphorylated form of this peptide S6K-HM was bound to an streptavidin- coated Sensor chip (SA) (12 response units, RU). 30 μl of wild type or the indicated mutant GST-PDK1 were injected at a flow rate of 30μl/min, in buffer HBS-P (10 mM HEPES pH 7.4, 0.15M NaCl, 0.005% (by vol) polysorbate-20) supplemented with 1 mM DTT. Specific interactions between S6K-pHM and PDK1 proteins were obtained between the concentration range of 2-2150 nM PDK1. Steady state binding was

determined at each concentration. Dissociation of PDK1 from the phosphopeptide was monitored over a 1min period. Regeneration of the sensor chip surface was performed with 10 \(\pi\)µl injections of 0.05% SDS. As previously found for PDK1 binding to PIFtide [Biondi et al., 2000], the interaction data obtained using BiaCore did not fit to simple 1:1 interaction model. Apparent Kd values were estimated from the concentration of PDK1 which gives 50% of maximal response, which was obtained empirically using GST-PDK1[T148A] (RUmax=435). For all PDK1 construct tested, the off rates for S6Kp-HM were high in comparison to those of PIFtide binding with the time taken for 50% dissociation to occur for S6K-pHM is 30s compared to 1000s for PIFtide. This could account for the overall approximately 100-fold lower affinity of wild type PDK1 for S6K-pHM in comparison to PIFtide.

15 Data collection, structure solution, and refinement

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Data on PDK1 crystals were collected at the European Synchrotron Radiation Facility (Grenoble, France) beamline ID14-EH1, using an ADSC Q4 CCD detector. The temperature of the crystals was maintained at 100K using a nitrogen cryostream. Data were processed using the HKL package [Otwinowski and Minor, 1997], statistics are shown in Table I.

The structure of PDK1 was solved by molecular replacement with AMoRe [Navaza, 1994] using the structure of PKA in complex with an inhibitory peptide as a search model (PDB entry 1YDB), against 8-4 Ådata. A single, well separated solution was found with an R-factor of 0.479 (correlation coefficient = 0.428). The structure was automatically built using warpNtrace [Perrakis et al., 1999], which found 262 of a possible 309 residues, giving an initial protein model with R=0.293 (Rfree=0.318) after simulated annealing in CNS [Brunger et al., 1998]. Iterative protein

building in O [Jones et al., 1991] together with refinement in CNS, which included incorporation of a model for ATP, the phosphoserine in the activation loop, solvent molecules and a key sulphate molecule, resulted in a final model with R=0.195 (Rfree=0.222). No electron density was observed for residues 51-70 (the N-terminus of the construct) and 233-236 (the tip of the activation loop). All figures were made with PyMOL (http://www.pymol.org).

Table I

ATP

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Details of data collection & structure refinement for the PDK1 kinase domain. Values between brackets are for the highest resolution shell. All measured data were included in structure refinement.

	Wave length ()	0.933
15	Space group	P3 ₂ 21
	Unit cell ()	a=123.01, b=123.01, c=47.62
	Resolution ()	25-2.0 (2.07-1.0)
	Observed reflections	77315
	Unique reflections	27643
20	Redundancy .	2.8 (2.5)
	Completeness(%)	98.0 (93.5)
	Rmerge	0.091 (0.454)
	I/ sigma I	7.3 (2.0)
	R _{free} reflections	579
25	R _{cryst}	0.195
	R_{free}	0.222
	Number of groups	•
	°°Protein residues	71-359
	°°Water	200

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	SO ₄	5
	Glycerol	. 8
	Wilson B (2)	22.4
•	Protein	25.6
5	Water	35.7
	< B > ATP	38.8
	RMSD from ideal geometry	
	Bond lengths ()	0.005
	Bond angles (°)	1.34
10	Main chain B (2)	1.5.

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Example 2: Co-ordinates for PDK1fragment with all alternate side chains.

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REMARK coordinates from restrained individual B-factor refinement
     REMARK refinement resolution: 25.0 - 2.0 A
     REMARK starting r= 0.1972 free_r= 0.2220
                      r= 0.1954 free_r= 0.2224
     REMARK final
     REMARK B rmsd for bonded mainchain atoms= 1.501 target= 1.5 REMARK B rmsd for bonded sidechain atoms= 2.235 target= 2.0
     REMARK B rmsd for angle mainchain atoms= 2.347 target= 2.0 REMARK B rmsd for angle sidechain atoms= 3.302 target= 2.5
     REMARK rweight= 0.0900 (with wa= 1.29263)
     REMARK target= mlf steps= 30
     REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
     gamma= 120
     REMARK parameter file 1 : /dd1/david/projects/PDK1 new/CNS/prot.par
    REMARK parameter file 2 : /ddl/david/projects/PDK1_new/CNS/atp.par
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
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     REMARK parameter file 4 : CNS_TOPPAR:ion.param

REMARK parameter file 5 : /ddl/david/projects/PDK1_new/CNS/glycerol.par
     REMARK molecular structure file: ../generate/alternate.mtf
     REMARK input coordinates: ../minimize/minimize.pdb
     REMARK reflection file= ../../1/hkl/cns.hkl
     REMARK ncs= none
     REMARK B-correction resolution: 6.0 - 2.0
     REMARK initial B-factor correction applied to fobs :
              B11= -2.766 B22= -2.766 B33=
                                                  5.532
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     REMARK
              B12= -0.375 B13= 0.000 B23=
     REMARK
                                                   0.000
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
     REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
     REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
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     REMARK theoretical total number of refl. in resol. range:
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     REMARK number of unobserved reflections (no entry or |F|=0):
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     CRYST1 123.013 123.013
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     MOTA
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	ATOM .	13	С	PRO A	72	57.527	-6.208	3.673	1.00	63.94	A
	ATOM	14	0	PRO A	72	56.710	-6.451	4.561	1.00	64.11	A
	ATOM	15	N	ALA A	73	57.341	-5.268	2.753	1.00	61.57	Α
	ATOM	16	CA	ALA A	73	56.133	-4.454	2.708	1.00	58.74	Α
5	ATOM	17	CB	ALA A	73	56.438	-3.030	3.165	1.00	58.05	. A
	ATOM	18	С	ALA A	73	55.626	-4.448	1.271	1.00	56.78	Α
	ATOM	19	0	ALA A	73	56.347	-4.834	0.349	1.00	56.95	A
	ATOM	20	N	PRO A	74	54.372	-4.024	1.057	1.00	54.15	Α
	ATOM	21	CD	PRO A	74	53.335	-3.610	2.018	1.00	53.31	Α
10	ATOM	22	CA	PRO A	74	53.856	-4.003	-0.314	1.00	52.54	Α
	ATOM	23	CB	PRO A	74	52.474	-3.375	-0.148	1.00	52.86	A
	ATOM	24	CG	PRO A	74	52.067	-3.824	1.226	1.00	52.88	A
	ATOM	25	С	PRO A	74	54.772	-3.167	-1.204	1.00	50.08	A.
	ATOM	26	0	PRO A	74	55.559	-2.361	-0.708	1.00	49.96	Α
15	ATOM	27	N	ALA A	75	54.680	-3.366	-2.514	1.00	47.58	Α
	ATOM	28	CA	ALA A	75	55.503	-2.602	-3.446	1.00	44.69	A
	ATOM	29	CB	ALA A	75	55.312	-3.121	-4.870		46.14	A
	ATOM	30	C	ALA A	75	55.100	-1.134	-3.371		41.55	A
	ATOM	31	ō	ALA A	75	53.947	-0.813	-3.086		41.01	A
20	MOTA	32	N	LYS A	76	56.053	-0.245	-3.619		38.31	A
20	ATOM	33	CA	LYS A	76	55.781	1.184	-3.588		35.72	
	ATOM	34	CB	LYS A	76	57.053	1.957	-3.930		37.70	
	ATOM	35	CG ·	LYS A	76	57.123	3.356	-3.350	1.00	40.99	A
•	ATOM	36	CD	LYS A	76	57.262	3.316	-1.836		40.04	Α
25	ATOM	37	CE	LYS A	76	57.511	4.705	-1,277	1.00	42.08	Α
	ATOM	38	NZ	LYS A	76	57.681	4.695	0.202	1.00	42.99	A
	ATOM	39	C	LYS A	76	54.708	1.467	-4.638	1.00	32.65	Α
	ATOM	40	Ö	LYS A	76	54.814	1.005	-5.770		31.41	A
	ATOM	41	N.	LYS A	77	53.668	2.207	-4.270	1.00	28.59	A
30	ATOM	42	CA	LYS A	77	52.619	2.517	-5.232	1.00	25.72	Α
30	ATOM	43	CB	LYS A	77	51.316	2.865	-4.509	1.00	26.22	Α
	ATOM	44	CG	LYS A	.77	50.796	1.731	-3.631	1.00	27.15	A
	ATOM	45	CD	LYS A	77	49.487	2.089	-2.967	1.00	26.80	A
	ATOM	46	CE	LYS A	77	49.136	1.091	-1.870	1.00	27.31	Α
35	ATOM	47	NZ	LYS A	77	48.998	-0.296	-2.380	1.00	27.17	Α
	ATOM	48	C	LYS A	77	53.053	3.668	-6.137	1.00	24.67	A
	ATOM .	49	.0	LYS A	77	54.010	4377	-5.829	1.00	21.60	Α
	ATOM	50	N	ARG A	78	52.351	3.838	-7.254	1.00	23.66	Α
	ATOM	51	CA	ARG A	78	52.662	4.897	-8.211	1.00	26.14	A
40	ATOM	52	СВ	ARG A	78	53.574	4.344	-9.318	1.00	28.57	A
	ATOM	53	CG	ARG A	78	53.017	3.139	-10.050	1.00	34.78	A
	ATOM	54	CD	ARG A	78	54.092	2.465	-10.896	1.00	40.96	Α
	ATOM	55	NE	ARG A	78	53.560	1.364	-11.700	1.00	48.93	A
	ATOM	56	CZ	ARG A	78	52.985	0.270	-11.203	1.00	52.58	Α
45	ATOM	57	NH1	ARG A	78	52.860	0.113	-9.889	1.00	54.60	Α
	ATOM	58		ARG A	78	52.530		-12.022	1.00	54.09	A
	ATOM	59	С	ARG A	78	51.382	5.488	-8.803	1.00	23.76	Α.
	ATOM	60	0	ARG A	78	50.311	4.888	-8.706	1.00	24.25	A
	ATOM	61	N	PRO A	79	51.475	6.676	-9.428	1.00	21.76	A
50	ATOM .	62	CD	PRO A	79	52.691	7.475	-9.668	1.00	20.82	Α
	ATOM	63	CA	PRO A	79	50.301	7.325	-10.021	1.00	21.96	Α
	ATOM	64	СВ	PRO A	79	50.910	8.481	-10.816	1.00	22.27	A
	ATOM	65	CG	PRO A	79	52.124	8.831	-10.014	1.00	22.12	A
	ATOM	66	С	PRO A	79	49.446	6.413	-10.903	1.00	22.86	Α
55	ATOM	67	0	PRO A	79	48.213		-10.842	1.00	20.52	A
	ATOM	68	N	GLU A	80	50.103		-11.714		21.87	
	ATOM	69	CA	GLU A	80	49.403	4.685	-12.628		22.99	Α
	ATOM	70	CB	GLU		50.393	3.994 -1		0.50 25	5.24	AC1
	ATOM	71	CG	GLU		51.230	2.907 -1	12.925	0.50 28	3.75	AC1

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2.224 -13.913
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     ATOM
              73
                   OE1 GLU
                               80 53.072
                                                                         AC1
                                            1.015 -14.172
                                                            0.50 32.83 AC1
     ATOM
              74
                   OE2 GLU
                               80 51.969
                                              3.631 -11.912
                                                               1.00 22.09
     ATOM
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                       GLU A
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                                    48.556
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                               81
                                                                                    Α
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                                                                                    Α
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                                                  4.934
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                               82
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                                                                                    Α
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                                                                                    Α
     ATOM
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                                                                                    Α
                   CD2 PHE A
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                                        47.520
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                                                                                    Α
20
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                   CE1 PHE A
                               82
              92
                   CE2
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                                                                                    Α
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              95
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                                                  5.792 -10.411
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25
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                                                                                    Α
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                       LYS A
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                                                                  1.00 22.02
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                       LYS A
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                                                  6.326 ~12.550
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                                        38.974
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                       LYS A
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                                                                  1.00 38.10
                                                                                    Α
30
                       LYS A
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     ATOM
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                                                                  1.00 43.33
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                                                  7.086 -13.043
                                                                                    Α
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                                                                  1.00 20.98
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                                                                  1.00 19.99
                                                                                    A
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                                        42.513
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                       PHE A
                               84
     MOTA
                   Ν
                                                                                    Α
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                               84
35
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             107
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                                                                                    Α
              108
                       PHE A
                               84
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                                                 10.741
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                   CD1 PHE A
     ATOM
             109
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                                                                  1.00 19.66
                                                                                    Α
                                                 11.183
                   CD2 PHE A
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     ATOM
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                                                                  1.00 18.09
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40
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                   CE1 PHE A
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     MOTA
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     ATOM
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                                                                  1.00 16.80
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45
     ATOM
                       GLY A
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                                                                                    Α
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                                                                                    Α
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                                                 13.673
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                                                                                    Α
                                                                  1.00 18.26
                                                                                    Α
                       LYS A
                                        37.571
                                                 15.064
                                                         -8.278
     MOTA
             121
                   CA
                               86
                                                                  1.00 19.00
                                        36.133
                                                         -7.812
                                                                                    Α
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     ATOM
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                               86
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                   CB
                                                 14.660
                                                                                    A
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                                                         -6.481
                                                                  1.00 21.55
     MOTA
              123
                   CG
                       LYS A
                               86
                                        34.368
                                                 14.981
                                                         -6.066
                                                                  1.00 26.48
                                                                                    Α
                               86
     ATOM
             124
                   CD
                       LYS A
                                                                                    Α
                       LYS A
                               86
                                        33.994
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                                                                  1.00 31.92
     ATOM
             125
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                                                                                    Α
                                                                  1.00 35.36
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                                                 14.457
                                                         -4.412
     MOTA
             126
                   NZ
                       LYS A
                                                         -7.202
                                                                  1.00 18.57
                                                                                    Α
                                        38.523
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                       LYS A
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                               86
                       LYS A
     ATOM
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                                                                                    A
                       ILE A
                               87
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     ATOM
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                   N
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                                                 17.554
                                                         -6.256
                                                                  1.00 18.26
     ATOM
             130
                       ILE A
                               87
                   CA
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	MOTA	131	CB	ILE	Α	87		39.994	18.952	-6.772	1.00 19.60	Α
•	ATOM	. 132	CG2	·ILE	Α	87		40.593	19.786	-5.628	1.00 18.73	Α
	ATOM	133		ILE		87		40.968	18.786	-7.945	1.00 21.16	A
	ATOM	134		ILE		87		41.412	20.087	-8.588	1.00 25.26	A
-		135	CDI	ILE		87		38.731	17.709	-4.997	1.00 19.67	A
5	ATOM											
	ATOM	136	0	ILE		87		37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU		88	•	39.240	17.229	-3.867	1.00 19.15	A
	MOTA	138	CA	LEU	A	88		38.508	17.324	-2.611	1.00 20.68	A
	MOTA	139	CB	LEU	Α	88		38.870	16.151	-1.700	1.00 19.97	A
10	MOTA	140	CG	LEU	Α	88		38.529	14.759	-2.237	1.00 19.24	A
	ATOM	141		LEU		88		39.090	13.692	-1.311	1.00 21.41	Α
	ATOM	142		LEU		88		37.029	14.622	~2.359	1.00 18.84	A
	ATOM	143	C	LEU		88		38.815	18.632	-1.901	1.00 23.11	A
								37.999	19.146	-1.139	1.00 25.10	A
	MOTA	144	O _i	LEU		88						A
15	ATOM	145	N	GLY		89		39.997	19.174	-2.149	1.00 24.09	
	MOTA	146	CA	GLY		89	•	40.367	20.418	-1.507	1.00 24.27	A
	MOTA	147	С	GLY	A	89		41.658	20.954	-2.078	1.00 25.47	A
	ATOM	148	0	GLY	Α	89		42.445	20.202	-2.666	1.00 22.19	A
	ATOM	149	N	GLU	Α	90		41.870	22.254	-1.906	1.00 26.22	Α
20	ATOM	150	CA	GLU		90		43.064	22.924	-2.404	1.00 29.96	A
20	ATOM	151	CB	GLU		90		42.698	23.814	-3.596	1.00 30.75	Α
		152	CG	GLU		90		42.267	23.038	-4.831	1.00 34.32	Α
	ATOM		CD	GLU		90		41.711	23.930	-5.927	1.00 38.27	A
	ATOM	153						40.590	24.456	-5.764	1.00 40.57	A
	MOTA	154	OE1			90					1.00 40.90	A
25	ATOM	155	OE2			90		42.398	24.110	-6.952		A
	ATOM	156	С	\mathtt{GLU}		90		43.711	23.768	-1.313	1.00 30.68	
	ATOM	157	0	${\tt GLU}$	Α	90		43.049	24.574	-0.668	1.00 32.83	A
	ATOM	158	N	GLY	Α	91		45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY	Α	91		45.724	24.332	-0.104	1.00 29.40	A
30	ATOM	160	С	GLY	Α	91		46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY		91		46.894	25.130	-2.028	1.00 28.16	Α
	ATOM	162	N	SER		92		47.605	25.870	-0.029	1.00 28.30	A
	ATOM	163	CA	SER		92		48.653	26.681	-0.633	1.00 30.50	A
						92		49.165	27.717	0.370	1.00 32.43	Α
~~	ATOM	164	CB	SER				49.520	27.099	1.593	1.00 40.94	А
35	ATOM	165	OG	SER		92				-1.164	1.00 29.77	A
	MOTA	166	С	SER		92		49.815	25.843		1.00 25.77	Ä
	ATOM	167	0	SER		92		50.456	26.221	-2.143		A
	MOTA	168	N	PHE	A	93		50.087	24.703	-0.536	1.00 27.65	•
	ATOM	169	CA	PHE	Α	93		51.185	23.855	-0.995	1.00 26.34	A
40	ATOM	170	CB	PHE	Α	93		52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Α	93		52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	Α	93		52.283	25.909	1.392	1.00 29.96	A
	ATOM	173		PHE		93		53.949	25.613	-0.308	1.00 31.38	A
	ATOM	174		PHE		93		52,779	27.181	1.665	1.00 32.69	A
15				PHE		93		54.452	26.883	-0.044	1.00 32.63	A,
45	ATOM	175						53.864	27.670	0.945	1.00 31.81	• A
	MOTA	176	CZ	PHE		93				-1.365	1.00 25.39	A
	MOTA	177	С	PHE		93		50.759	22.445		1.00 24.59	A
	MOTA	178	0	PHE		93		51.601	21.559	-1.522		A
	ATOM	179	N	SER		94		49.457	22.235	-1.519	1.00 23.63	
50	ATOM	180	CA	SER	Α	94		48.965	20.912	-1.860	1.00 21.43	A
	ATOM	181	CB	SER	Α	94		49.017	20.013	-0.628	1.00 21.42	Α
	ATOM	182	OG	SER		94		48.091	20.475	0.340	1.00 21.19	. A
	ATOM	183	C	SER		94		47.539	20.925	-2.378	1.00 19.82	A
	ATOM	184	ŏ	SER		94		46.795	21.882	-2.173	1.00 18.76	A
55		185		THR		95		47.174	19.832	-3.038	1.00 19.38	A
55	ATOM		N Cn			95		45.840	19.637	-3.580	1.00 17.98	A
	ATOM	186	CA	THR				45.818	19.818	-5.110	1.00 19.25	A
	ATOM	187	CB	THR		95				-5.434	1.00 13.23	A
	ATOM	188		THR		95		46.196	21.162		1.00 22.04	A
	MOTA	189	CG2	THR	A	95		44.421	19.549	-5.661	1.00 17.01	. А
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			_		_		_					
	ATOM	190	C,	THR	A 9	95	45.455	18.201	-3.243	1.00	18.61	A
	ATOM	191	0	THR	A 9	95	46.212	17.264	-3.524	1.00	17.10	A
	ATOM	192	N	VAL		96	44.295	18.024	-2.623		16.53	
												A
	ATOM	193	CA	VAL	A 9	96	43.845	16.685	-2.266		16.05	A
5	MOTA	194	CB	VAL	A 9	96	43.170	16.672	-0.886	1.00	16.32	A
	ATOM	195	CG1	VAL	Α (96	42.741	15.249	-0.532		18.02	A
		196		VAL				17.206	0.168			
	ATOM					96	44.145				16.69	A
	MOTA	197	С	VAL	A S	96	42.875	16.207	-3.335		16.42	Α
	ATOM	198	0	VAL	A 9	96	41.906	16.892	-3.665	1.00	16.47	A
10	ATOM	199	N	VAL	Δ (97	43.157	15.033	-3.888		16.80	A
10												
	MOTA	200	CA	VAL		97	42.338	14.471			16.72	A
	ATOM	201	CB	VAL	A S	97	43.153	14.354	-6.255	1.00	18.43	A
	ATOM	202	CG1	VAL	A 9	7	42.249	13.927	-7.404	1.00	19.69	A
	ATOM	203	CG2	VAL .	2 (97	43.831	15.685	-6.569	1.00	17.84	A
16									-4.583		16.77	A
15	ATOM	204	С	VAL		7	41.812	13.091				
	MOTA	205	0	VAL	A 9	97	42.532	12.270	-4.014	1.00	17.13	A
	MOTA	206	N	LEU	A 9	98	40.545	12.845	-4.895	1.00	16.62	Α
	ATOM	207	CA	LEU	Z	8	39.947	11.548	-4.624	1.00	17.04	·A
											16.89	· A
	ATOM	208	СВ	LEU		8	38.424	11.633	-4.743			
20	MOTA	209	CG	LEU	A 9	98	37.635	10.342	-4.508	1.00	19.46	A
	ATOM	210	CD1	LEU	A 9	8	37.990	9.762	-3.146	1.00	20.07	Α
	ATOM	211	CD2	LEU		8	36.143	10.627	-4.588	1 00	17.93	A
								10.597	-5.677		17.38	A
	MOTA	212	C	LEU		8	40.512					
	MOTA	213	0	LEU	A 9	. 8	40.527	10.920	-6.863		18.60	A
25	ATOM	214	N	ALA	A 9	9	40.995	9.438	-5.246	1.00	17.13	'A
	ATOM	215	CA	ALA	A (9	41.570	8.466	-6.168	1.00	18.42	A
				ALA		9	43.090	8.524	-6.105		14.76	A
	ATOM	216	CB									
	ATOM	217	С	ALA		9	41.102	7.055	-5.848		21.40	A
	MOTA	218	0	ALA	A 9	9	40.941	6.691	-4.679	1.00	22.52	A
30	ATOM	219	N	ARG	A 10	00	40.878	6.261	-6.888	1.00	19.77	A
50		220		ARG			40.459	4.884	-6.693		20.85	A
	ATOM		CA									
	ATOM	221	CB	ARG			39.202	4.585	-7.518		24.22	A
	ATOM	222	CG	ARG	A 10	0	38.608	3.205	-7.256	1.00	31.78	A
	MOTA	223	CD	ARG	A 10	00	37.326	2.979	-8.048	1.00	36.24	A
35	ATOM	224	NE	ARG			36.213	3.818	-7.594	1.00	41.40	A
33											42.05	A
	MOTA	225	cz	ARG			35.566	3.662	-6.439			
	ATOM	226	NH1	ARG	A 10	00	35.912	2.696	-5.598	1.00	40.67	A
	ATOM	227	NH2	ARG	A 10	0	34.559	4.468	-6.128	1.00	43.65	A
	ATOM	228	С	ARG			41.613	3.985	-7.129	1.00	18.63	Α
40		229	o	ARG			42.078	4.065	-8.271		19.49	A
40	ATOM											A
	MOTA	230	N	GLU			42.102	3.157	-6.212		16.43	
	ATOM	231	CA	GLU	A 10)1	43.196	2.246	-6.533	1.00	16.11	A
	ATOM	232	СВ	GLU	A 10	1	43.774	1.637	-5.248	1.00	16.79	Α
	ATOM		CG	GLU			44.917	0.657	-5.488	1.00	16.51	A
4~							45.501		-4.200		18.20	A
45	ATOM	234		GLU								
	MOTA	235	OE1	GLU	A 10	1	44.733		3.239		18.32	Α
	ATOM	236	OE2	GLU	A 10	1	46.725	-0.132	-4.150	1.00	17.14	A
	ATOM	237	С	GLU			42.625	1.152	-7.442	1.00	17.92	Α
							41.681	0.462	-7.069		18.02	Α
	ATOM	238	0	GLU .								
50	ATOM	239	N	LEU			43.198	1.002	-8.632		19.06	Α
	ATOM	240	CA	LEU	A 10	2	42.718	0.025	-9.607	1.00	20.71	A
•	ATOM	241	СВ	LEU	A 10	2	43.569	0.097	-10.878	1.00	23.42	Α
		242	CG	LEU			43.531		-11.642		25.30	A
	ATOM											
	ATOM	243		LEU			44.577		-12.748		27.88	A
55	ATOM	244	CD2	LEU	A 10	12	42.140	1.647	-12.214		26.79	A
	ATOM	245	С	LEU	A 10	2	42.671	-1.418	-9.125	1.00	21.62	Α
	ATOM	246	ō	LEU			41.668	-2.103	-9.305	1.00	21.09	A
								-1.874	-8.507		19.38	A
	MOTA	247	N	ALA			43.753					
	ATOM	248	CA	ALA	A 10	13	43.836	-3.249	-8.035	1.00	20.87	A

	ATOM ATOM	249 250	CB C	ALA	A	103 103		45.284 42.919	-3.571 -3.629	-7.671 -6.872	1.00 19.23 1.00 19.92	A A	
	ATOM	251 252	0			103		42.703	-4.815	-6.628	1.00 20.38	A	
5	ATOM ATOM	252	N CA			104 104		42.361 41.517	-2.643	-6.175	1.00 18.12	A	
5	ATOM	254	CB			104		42.212	-2.927 -2.484	5.018	1.00 17.15	A	
	ATOM	255		THR				42.456	-1.070	-3.717 -3.773	1.00 19.54 1.00 19.26	A	
	ATOM	256		THR				43.536	-3.219	-3.529	1.00 13.20	A A	
	ATOM	257	C			104		40.159	-2.247	-5.026	1.00 17.02	A	
10	ATOM	258	Õ			104		39.259	-2.648	-4.285	1.00 13.44	A	
	ATOM	259	N			105		40.034	-1.207	-5.847	1.00 19.65	A	
	ATOM	260	CA			105		38.819	-0.400	-5.967	1.00 19.37	A	
	ATOM	261	СВ	SER		105		37.598	-1.304	-6.173	0.50 21.81	AC	1
	ATOM	262	OG	SER		105		36.431	-0.539	-6.412	0.50 23.01	AC:	
15	ATOM	263	С	SER	A	105		38.644	0.447	-4.701	1.00 18.99	A	
	ATOM	264	0	SER	Α	105		37.602	1.070	-4.488	1.00 18.66	A	
	MOTA	265	N	ARG	Α	106		39.674	0.468	-3.861	1.00 16.84	A ·	•
	ATOM	266	CA	ARG	Α	106		39.655	1.267	-2.634	1.00 16.21	A	
	ATOM	267	CB			106		40.827	0.886	-1.723	1.00 16.41	Α	
20	ATOM	268	CG			106		40.619	-0.367	-0.906	1.00 15.49	A	
	ATOM	269	CD			106		41.887	-0.755	-0.170	1.00 17.43	A	
	MOTA	270	NE			106		41.620	-1.792	0.824	1.00 20.47	Α	
	ATOM	271	CZ			106		42.548	-2.568	1.371	1.00 20.24	· A	
25	ATOM	272		ARG			,	43.821	-2.433	1.017	1.00 17.80	A	
25	ATOM	273 274		ARG		106		42.198	-3.468	2.285	1.00 20.14	A	
	ATOM ATOM	275	С 0			106		39.785 40.514	2.746 3.103	-2.981 -3.902	1.00 17.37 1.00 17.75	A A	
	ATOM	276	N	GLU				39.085	3.599	-2.240	1.00 17.75	A	
	ATOM	277	CA	GLU				39.156	5.039	-2.461	1.00 20.80	A	
30	ATOM	278	CB	GLU				37.779	5.694	-2.337	1.00 22.93	A	
	ATOM	279	CG	GLU				36.711	5.171	-3.269	1.00 30.87	A	
	ATOM	280	CD	GLU				35.431	5.975	-3.148	1.00 32.40	A	
	ATOM	281		GLU				35.262	6.939	-3.923	1.00 33.74	A	
	ATOM	282	OE2	GLŲ	A	107		34.608	5.654	-2.263	1.00 36.00	A	
35	ATOM	283	С.	GLU	A	107		40.053	5.678	-1.410	1.00 18.93	A	
	MOTA	284	0	GLU	Α	107		39.891	5.427	-0.220	1.00 19.21	Α	
	MOTA	285	N	TYR				40.988	6.507	-1.852	1.00 16.70	A.	
	ATOM	286	CA	TYR				41.883	7.209	-0.942	1.00 15.86	A	
	ATOM	287	CB	TYR				43.325	6.728	-1.104	1.00 15.30	A	
40	ATOM	288	CG	TYR				43.593	5.328	-0.612	1.00 16.33	A	
	ATOM	289		TYR				43.765	5.066	0.746	1.00 16.36	A	
	ATOM	290		TYR				44.046	3.769	1.201	1.00 18.48	A	
	ATOM ATOM	291 292		TYR TYR				43.701 43.980	4.268 2.981	-1.511 -1.075	1.00 13.25 1.00 17.28	. A	
45	ATOM	292		TYR				43.960		0.276		A	
73	ATOM	294	OH	TYR				44.132	1.461	0.688	1.00 19.17	A A	
	ATOM	295	C	TYR				41.850	8.687	-1.292	1.00 15.38	A	
	ATOM	296	o	TYR				41.560	9.058	-2.431	1.00 15.22	A	
	ATOM	297	N	ALA				42.132	9.528	-0.306	1.00 14.61	A	
50	ATOM	298	CA	ALA				42.207	10.957	-0.539	1.00 14.30	A	
	ATOM	299	СВ	ALA				41.671	11.726	0.661	1.00 14.78	Α .	
	ATOM	300	С	ALA				43.713	11.136	-0.667	1.00 16.79	Α	
	ATOM	301	0	ALA				44.450	10.983	0.317	1.00 16.52	A	
	MOTA	302	N	ILE	Α	110		44.182	11.410	-1.881	1.00 14.80	A	
55	MOTA	303	CA	ILE	A	110		45.609	11.574	-2.093	1.00 15.80	A	
	MOTA	304	CB	ILE				46.065	10.863	-3.396	1.00 16.85	Α	
	ATOM	305	CG2					47.550	11.098	-3.632	1.00 16.80	Α	
	ATOM	306		ILE				45.774	9.358	-3.284	1.00 17.76	A	
	ATOM	307	CD1	ILE	A	110		46.308	8.513	-4.437	1.00 16.07	A	

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	MOTA	308	С	ILE A	110	46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE F	110	45.534	13.813	-2.976	1.00 16.24	·A
	ATOM	310	N	LYS F	111	46.846	13.435	-1.177	1.00 16.15	А
	ATOM	311	CA	LYS F	111	47.326	14.808	-1.100	1.00 17.20	Α
5	ATOM	312	CB	LYS F	111	47.700	15.176	0.344	1.00 17.41	A
	ATOM	313	CG	LYS P	111	48.350	16.547	0.464	1.00 20.71	Α
	MOTA	314	CD	LYS A	111	48.585	16.971	1.910	1.00 24.25	A
	ATOM	315	CE	LYS A	111	47.288	17.381	2.598	1.00 29.46	A
	MOTA	316	NZ	LYS A	111	47.516	17.866	4.000	1.00 30.50	A
10	MOTA	317	С	LYS A	111	48.551	14.890	-1.994	1.00 16.41	A
	MOTA	318	0	LYS A	111	49.509	14.137	-1.813	1.00 18.20	A
	ATOM	319	N	ILE A	112	48.509	.15.798	-2.963	1.00 15.87	Ά
	MOTA	320	CA	ILE A	112	49.606	15.967	-3.907	1.00 17.28	A
•	MOTA	321	CB	ILE A	112	49.079	15.911	-5.358	1.00 16.43	A
15	ATOM	322	CG2	ILE A	. 112	50.235	15.998	-6.341	1.00 15.12	A
	ATOM	323	CG1			48.293	14.609	-5.565	1.00 16.82	A
	MOTA	324	CD1	ILE A	. 112	47.580	14.511	-6.904	1.00 18.47	Α
	ATOM	325	С	ILE A	112	50.307	17.301	-3.663	1.00 19.03	A
	ATOM	326	0	ILE A	112	49.669	18.350	-3.635	1.00 19.15	Α
20	ATOM	327	N	LEU A	113	51.622	17.245	-3.472	1.00 20.22	. A
	MOTA	. 328	CA	LEU A	113	52.416	18.442	-3.214	1.00 22.36	Α
	MOTA	329	CB	LEU A	113	52.995	18.397	-1.794	1.00 22.13	A
	ATOM	330	CG	LEU A	113	52.042	18.063	-0.646	1.00 22.46	A
	ATOM	331		LEU A		51.866	16.557	-0.553	1.00 23.81	A
25	MOTA	332	CD2	LEU A	113	52.603	18.595	0.660	1.00 23.68	A
	ATOM	333	С	LEU A	113	53.560 ·	18.547	-4.215	1.00 23.37	A
	MOTA	334	0	LEU A	113	54.300	17.586	-4.424	1.00 23.11	A
	ATOM	335	N	GLU A	114	53.706	19.714	-4.834	1.00 23.88	A
	MOTA	336	CA	GLU A	114	54.771	19.920	-5.806	1.00 26.00	A
30	ATOM	337	CB	GLU A	114	54.435	21.111	-6.706	1.00 27.74	A
	MOTA	338	CG	GLU A	114	55.533	21.452	-7.696	1.00 35.07	A
	ATOM	339	CD	GLU A		55.220	22.696	-8.497	1.00 39.24	Α
	MOTA	340	OE1	GLU A	114	54.808	23.703	-7.885	1.00 41.45	A
	MOTA	341	OE2	GLU A	114	55.395	22.670	-9.736	1.00 44.05	A
35	MOTA	342	С	GLU A	114	56.087	20.163	-5.067	1.00 24.37	A
	ATOM	343	0	GLU A	114	56.186	21.071	-4.238	1.00 24.43	A
	MOTA	344	N '	LYS A	115	57.096	19.350	-5.360	1.00 24.10	A
	ATOM	345	CA	LYS A	115	58.376	19.493	-4.678	1.00 24.93	A
	MOTA	346	СВ	LYS A	115	59.339	18.373	-5.103	1.00 23.72	A
40	ATOM	347	CG	LYS A	115	59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD	LYS A	115	60.064	15.944	-4.743	1.00 21.92	A
•	ATOM	349	CE	LYS A	115	59.691	15.400	-6.117	1.00 22.42	A
	ATOM	350	ΝZ	LYS A		60.447	14.150	-6.448	1.00 19.71	A
	ATOM	351	С	LYS A	115	59.031	20.858	-4.868	1.00 26.87	A
45	MOTA	352	0	LYS A	115	59.492	21.469	-3.903	1.00 26.17	A
	ATOM ·	353	N	ARG A	116	59.058	21.348	-6.102	1.00 28.73	A
	ATOM	.354	CA	ARG A	116	59.678	22.638	-6.380	1.00 29.66	A
	ATOM	355	CB	ARG	116	59.533	22.980	-7.868	0.50 31.29	AC1
	ATOM	356	CG	ARG	116	60.047	24.361	-8.267	0.50 33.19	AC1
50	ATOM	357	CD	ARG	116	61.368	24.710	-7.590	0.50 35.13	AC1
	ATOM	358	NE	ARG	116	62.329	23.612	-7.618	0.50 36.42	AC1
	MOTA	359	CZ	ARG	116	63.510	23.648	-7.009	0.50 36.18	AC1
	ATOM	360	NH1	ARG	116	63.871	24.729	-6.332	0.50 36.12	AC1
	MOTA	361		ARG	116	64.324	22.602	-7.067	0.50 35.77	AC1
55	ATOM	362	С	ARG A	116	59.097	23.761	-5.519	1.00 29.70	A
	ATOM	363	0	ARG A	116	59.843	24.515	-4.889	1.00 29.16	A
	ATOM	364	N	HIS A		57.773	23.862	-5.472	1.00 27.22	Α
	ATOM	365	CA	HIS A		57.126	24.903	-4.681	1.00 26.33	A
	ATOM	366	СВ	HIS A		55.606	24.835	-4.848	1.00 28.41	A

	ATOM	367	CG	HIS	Α	117	54.881	26.005	-4.258	1.00 31.82	A
	ATOM	368	CD2	HIS	Α	117	55.309	27.249	-3.935	1.00 33.19	· A
	ATOM	369	ND1	HIS	Α	117	53.536	25.974	-3.961	1.00 34.30	A
	ATOM	370	CE1	HIS	Α	117	53.165	27.148	-3.480	1.00 34.58	A
5	ATOM	371	NE2	HIS	Α	117	54.222	27.940	-3.455	1.00 35.18	A
	ATOM	372	C	HIS	Α	117	57.477	24.780	-3.202	1.00 26.22	Α
	ATOM	373	0	HIS	Α	117	57.737	25.776	-2.534	1.00 25.67	A.
	ATOM	374	N	ILE	Α	118	57.469	23.554	-2.689	1.00 24.94	A
	ATOM	375	CA	ILE	Α	118	57.792	23.315	-1.285	1.00 23.94	А
10	ATOM	376	CB	ILE	Α	118	57.711	21.812	-0.952	1.00 23.50	А
	ATOM	377	CG2	ILE	A	118	58.374	21.533	0.389	1.00 23.76	· A
	ATOM	378	CG1	ILE	Α	118 '	56.246	21.362	-0.959	1.00 24.42	A
	ATOM	379	CD1	ILE	Α	118	56.066	19.858	-0.834	1.00 28.06	A
	ATOM	380	С	ILE	Α	118	59.195	23.821	-0.958	1.00 23.78	A
15	ATOM	381	0	ILE	Α	118	59.402	24.495	0.048	1.00 23.49	A
	ATOM	382	N	ILE	Α	119	60.153	23.489	-1.815	1.00 23.46	A
	ATOM	383	CA	ILE	Α	119	61.534	23.913	-1.619	1.00 25.13	A
	ATOM	384	CB	ILE	A	119	62.467	23.250	-2.664	1.00 24.25	Α
	ATOM	385	CG2	ILE			63.858	23.890	-2.617	1.00 22.47	A
20	ATOM	386	CG1	ILE	Α	119	62.540	21.738	-2.395	1.00 25.05	A
	ATOM	387	CD1	ILE	Α	119	63.327	20.945	-3.439	1.00 24.62	A
	MOTA	388	С	ILE			61.667	25.435	-1.705	1.00 25.96	A
	ATOM	389	0	ILE	Α	119	62.330	26.051	-0.872	1.00 24.78	Α
	ATOM	390	N	LYS	Α	120	61.028	26.039	-2.704	1.00 27.67	A
25	ATOM	391	CA	LYS	Α	120	61.100	27.489	-2.879	1.00 30.29	A
	ATOM	392	CB	LYS	Α	120	60.242	27.940	-4.060	1.00 32.34	A
	MOTA	393	CG	LYS	Α	120	60.674	27.407	-5.409	1.00 39.30	A
	MOTA	394	CD	LYS	Α	120	59.765	27.950	-6.512	1.00 45.19	A
	MOTA	395	CE ·	LYS	Α	120	58.294	27.636	-6.218	1.00 46.48	A
30	ATOM	396	NZ	LYS	Α	120	57.363	28.155	-7.252	1.00 46.49	A
	ATOM	397	С	LYS	Α	120	60.647	28.247	-1.638	1.00 30.89	A
	ATOM	398	0	LYS	A	120	61.303	29.198	-1.217	1.00 32.48	A
	MOTA	399	N	GLU	Α	121	59.527	27.825	-1.055	1.00 29.82	A
•	MOTA	400	CA	GLU			58.986	28.488	0.128	1.00 30.33	A
35	MOTA	401	CB	${ t GLU}$	Α	121	57.455	28.416	0.117	1.00 33.04	A
	ATOM	402	CG	GLU			56.794	29.021	-1.120	1.00 36.45	A
	ATOM	403	CD	GLU			57.221	30.456	-1.373	1.00 39.88	A
	ATOM	404		${\tt GLU}$			57.200	31.264	-0.420	1.00 40.53	A
	ATOM	405		GLU			57.573	30.778	-2.529	1.00 43.24	A
40	ATOM	406	С	GLÜ			59.511	27.930	1.451	1.00 30.37	A
	MOTA	407	0	GLU			58.946	28.204	2.513	1.00 31.24	A
	ATOM	408	N	ASN			60.588	27.151	1.390	1.00 29.03	A
	ATOM	409	CA	ASN			61.183	26.573	2.594	1.00 28.46	A
	ATOM	410	CB	ASN			61.836	27.673	3.436	1.00 31.28	A
45	MOTA	411	CG	ASN			62.945	28.395	2.698	1.00 34.12	A
	MOTA	412		ASN			62.697	29.143	1.754	1.00 35.57	· A
	MOTA	413		ASN			64.181 .		3.127	1.00 35.73	A
	MOTA	414	С	ASN			60.157	25.835	3.456	1.00 26.89	A
	ATOM	415	0	ASN			60.085	26.055	4.663	1.00 27.23	A
50	MOTA	416	N	LYS			59.375	24.955	2.842	1.00 23.99	A
	ATOM	417	CA	LYS			58.358	24.210	3.574	1.00 22.43	A
	ATOM	418	CB	LYS			57.031	24.248	2.810	1.00 21.97	A
	ATOM	419	CG	LYS			56.475	25.645	2.599	1.00 25.68	
c	ATOM	420	CD	LYS			56.253	26.354	3.927	1.00 27.54	A
55	ATOM	421	CE	LYS			55.822	27.796	3.716	1.00 31.30	A
	ATOM	422	NZ	LYS			55.756	28.540	5.004	1.00 33.21	. A
	ATOM	423	C	LYS			58.748	22.759	3.821	1.00 22.20	A A
	ATOM	424	0	LYS			57.924	21.960	4.264	1.00 22.50	
	ATOM	425	N	VAL	A	124	59.997	22.412	3.535	1.00 20.59	A

	ATOM	426	CA	VAL	A	124		60.439	21.039	3.730	1.00	20.25		A
	ATOM	427	СВ	VAL	Α	124		61.922	20.850	3.328	1.00	19.43	•	Α
	ATOM	428	CG1	VAL	A	124		62.346	19.407	3.573	1.00	18.69		A
	MOTA	429	CG2	VAL				62.104	21.195	1.853		18.21		Α
5	ATOM	430	С	\mathtt{VAL}	А	124		60.236	20.561	5.163	1.00	19.53		Α
	MOTA	431	0	VAL			·	59.841	19.418	5.385	1.00	20.02		Α
	MOTA	432	N	PRO	Α	125		60.513	21.422	6.159	1.00	20.01		Α
	ATOM	433	CD	PRO	A	125		61.178	22.738	6.118	1.00	18.69		Α
	MOTA	434	CA	PRO	Α	125		60.318	20.979	7.544	1.00	19.88		Α
10	ATOM	435	СВ	PRO				60.793	22.180	8.363	1.00	19.95		Α
	MOTA	436	CG	PRO	Α	125		61.839	22.805	7.479	1.00	18.85		Α
	ATOM	437	С	PRO	Α	125		58.848	20.642	7.824	1.00	19.76		Α
	MOTA	438	0	PRO	Α	125		58.544	19.700	8.550	1.00	16.99		Α
	MOTA	439	N	TYR	Α	126		57.947	21.418	7.235	1.00	18.98		Α
15	ATOM	440	CA	TYR	Α	126		56.516	21.220	7.435	1.00	21.97		Α
	ATOM	441	CB	TYR	Α	126		55.752	22.448	6.933		25.17		A
	MOTA	442	CG	TYR	Α	126		56.040	.23.690	7.748		30.98		A
	MOTA	443	CD1	TYR	A	126		55.438	23.886	8.991		33.95		A
	ATOM	444	CE1	TYR	Α	126		55.721	25.015	9.763		36.60		А
20	ATOM	445	CD2	TYR	Α	126		56.938	24.657	7.292		35.43		А
	ATOM	446	CE2	TYR				57.231	25.792	8.058		37.20		Α
	MOTA	447	CZ	TYR				56.618	25.962	9.291		37.40		A
	ATOM	448	ОН	TYR	Α	126		56.903	27.073	10.052		40.85		A
•	MOTA	449	С	TYR				55.990	19.956	6.762		21.35		A
25	ATOM	450	0	TYR	Α	126		55.265	19.175	7.383		20.49		Α
	ATOM	451	N	VAL				56.354	19.746	5.501		18.16		A
	ATOM	452	CA	VAL				55.892	18.562	4.790		17.58		Α
	ATOM	453	CB	VAL				56.308	18.596	3.308		17.45		Α
	MOTA	454		VAL				55.786	17.350	2.600		17.97		A
30	MOTA	455		VAL				55.751	19.850	2.641		14.90		A
	MOTA	456	С	VAL				56.459	17.306	5.448		18.39		A
	ATOM	457	0	VAL				55.769	16.298	5.583		18.14		Ą
	MOTA	458	N	THR				57.716	17.381	5.869		17.50		A
	ATOM	459	CA	THR				58.375	16.260	6.530		18.54		A
. 35	MOTA	460	CB	THR				59.861	16.586	6.805		18.01		A
	ATOM	461	OG1					60.537	16.804	5.559		21.14		A
	ATOM	462	CG2					60.536	15.446	7.545		17.95		A
	ATOM	463	C	THR				57.676	15.941	7.856		19.49		A
	MOTA	464	0	THR				57.438	14.776	8.179		18.76		A
40	ATOM	465	N	ARG				57.345	16.981	8.619		19.60 20.12		A
	ATOM	466	CA	ARG				56.673	16.804	9.904 10.621		21.33		A A
	ATOM	467	CB	ARG				56.534	18.144	12.023		28.02		A
	MOTA	468	CG	ARG				55.948	18.029 19.404	12.023		31.25		A
45	ATOM	469	CD	ARG				55.721						_
45	ATOM	470	NE	ARG				56.940	20.205	12.560 12.391		37.78 40.10		A A
•	ATOM	471	CZ	ARG	-			56.962	21.524	12.239		40.10		A
	ATOM	472		ARG				55.828	22.197	12.239		44.58		A
	ATOM	473		ARG				58.119	22.170 16.186	9.729		20.08		A ·
50	ATOM	474	С	ARG				55.288 54.891	15.305	10.496		20.40		A
50	ATOM	475	0	ARG GLU					16.654	8.724		18.79		A
	ATOM	476	N					54.553 53.222	16.125	8.454		20.10		A
	ATOM	477	CA	GLU GLU				52.638	16.749	7.183		19.92		A
-	MOTA	478	CB	GLU				52.638	16.749	6.708		27.85		A
55	ATOM	479 480	CG CD	GLU				50.581	16.933	5.707		29.72		A
55	ATOM	480 481		GLU .				51.216	17.528	4.814		33.46		A
	ATOM ATOM	481		GLU				49.339	16.996	5.807		30.74		A
		482 483	C C	GLU				53.301	14.615	8.295		19.81		A
	ATOM		0	GLU				52.553	13.875	8.935		18.37		A
	ATOM	484	J	OTTO	M	100		J2.JJ3	13.073	0.755	1.00	,,		• •

								Ca		•
	ATOM	485		ARG A 13:		54.219		7.447	1.00 20.41	· A
	ATOM	486			1	54.397		7.202	1.00 22.45	A
	MOTA	487				55.442	12.511	6.098	1.00 25.16	А
_	MOTA	.488				55.742	11.043	5.840	1.00 28.75	A
5	ATOM	489				56.736	10.837	4.708	1.00 33.75	А
	ATOM	490				57.020	9.415	4.520	1.00 40.07	A
	ATOM	491	CZ			57.756	8.915	3.532	1.00 43.07	A
	MOTA	492		1 ARG A 131		58.293	9.721	2.625	1.00 44.91	A
••	MOTA	493		2 ARG A 131		57.955	7.606	3.449	1.00 44.45	A
10	ATOM	494	С	ARG A 131		54.820	11.982	8.466	1.00 23.24	A
	ATOM	495	0	ARG A 131		54.241	10.948	8.804	1.00 23.86	· A
	ATOM	496	N	ASP A 132		55.831	12.497	9.160	1.00 21.99	A
	ATOM	497	CA	ASP A 132		56.318	11.850	10.370	1.00 22.04	A
	MOTA	498	CB	ASP A 132		57.570	12.564	10.888	1.00 23.72	Α
15	ATOM	499	CG	ASP A 132		58.750	12.442	9.932	1.00 27.77	A
	MOTA	500		1 ASP A 132		58.681	11.620	8.989	1.00 27.34	A
	ATOM	501	OD:	2 ASP A 132		59.753	13.163	10.128	1.00 28.70	A
	MOTA	502	С	ASP A 132		55.258	11.772	11.474	1.00 21.69	A
	ATOM	503	0	ASP A 132		55.077	10.723	12.092	1.00 22.75	A
20	MOTA	504	N	VAL A 133		54.551	12.868	11.725	1.00 19.54	A
	ATOM	505	CA	VAL A 133		53.525	12.843	12.759	1.00 18.52	A
	ATOM	506	CB	VAL A 133		52.908	14.244	12.990	1.00 19.26	А
	MOTA	507		l VAL A 133		51.708	14.135	13.918	1.00 18.79	Α
	ATOM	508	CG2	2 VAL A 133		53.953	15.180	13.604	1.00 18.80	A.
25	ATOM	509	С	VAL A 133		52.419	11.854	12.398	1.00 19.46	А
	ATOM	510	0	VAL A 133		52.073	10.991	13.200	1.00 19.94	A
	MOTA	511	N	MET A 134		51.878	11.957	11.187	1.00 19.15	A
	MOTA	512	CA	MET A 134		50.807	11.052	10.792	1.00 21.25	A
	ATOM	513	CB	MET A 134		50.309	11.381	9.383	1.00 17.34	Α
30	ATOM.	514	CG	MET A 134		49.615	12.730	9.302	1.00 20.00	Α
	ATOM	515	SD	MET A 134		48.643		7.798	1.00 24.21	A
	ATOM	516	CE	MET A 134		47.033	12.434	8.400	1.00 23.20	A
	ATOM	517	С	MET A 134		51.203	9.582	10.881	1.00 22.43	A
0.5	ATOM	518	0	MET A 134		50.384	8.741	11.249	1.00 23.82	Α
35	ATOM	519	N	SER A 135		52.454	9.273	10.556	1.00 23.09	Α
	ATOM	520	CA	SER A 135		52.939	7.895	10.615	1.00 26.13	A
	ATOM	521	CB	SER A 135		54.356	7.798	.10.039	1.00 26.17	A
	ATOM	522	OG	SER A 135		54.383	8.177	8.673	1.00 31.91	Α
40	ATOM	523	С	SER A 135		52.957	7.358	12.045	1.00 26.58	A
40	ATOM	524	0	SER A 135		52.926	6.148	12.261	1.00 26.42	Α
	ATOM	525	N	ARG A 136		53.014	8.261	13.018	1.00 25.65	Α
	ATOM	526	CA	ARG A 136		53.056	7.870	14.425	1.00 27.47	A
	ATOM	527	CB	ARG A 136		53.823	8.914	15.238	1.00 27.97	A
15	ATOM	528	CG	ARG A 136		55.283	9.082	14.857	1.00 32.00	A
45	ATOM	529	CD	ARG A 136		55.904	10.218	15.664	1.00 33.03	Α
	ATOM	530	NE	ARG A 136		55.602	10.073	17.084	1.00 36.11	· A
	ATOM	531	CZ	ARG A 136		55.867	10.990	18.007	1.00 39.74	, A
	ATOM	532		ARG A 136		56.449	12.132	17.661	1.00 40.55	A
50	ATOM	533		ARG A 136		55.540	10.769	19.276	1.00 36.72	A
50	ATOM	534	C	ARG A 136		51.667	7.709	15.036	1.00 26.38	A
	ATOM	535	0	ARG'A 136		51.516	7.121	16.106	1.00 27.06	A
	ATOM	536	N	LEU A 137		50.655	8.235	14.360	1.00 24.77	A
	ATOM	537	CA	LEU A 137		49.294	8.162	14.870	1.00 24.70	A
55	ATOM	538	CB	LEU A 137		48.483	9.363	14.371	1.00 24.52	A
رر	MOTA	539	CG	LEU A 137		49.050	10.760	14.662	1.00 26.67	A
	ATOM	540		LEU A 137		48.075	11.813	14.141	1.00 27.25	A
	ATOM	541		LEU A 137	٠	49.279	10.945	16.155	1.00 27.09	A
	ATOM	542	С	LEU A 137		48.592	6.868	14.473	1.00 25.20	A
	MOTA	543	0	LEU A 137		48.619	6.469	13.309	1.00 25.99	· А

	ATOM	544	N	ASP	A 138		47.971	6.218	15.451	1 00	21.89	70
•	ATOM	545	CA		A 138							A
							47.239		15.219		21.35	А
	ATOM	546	CB		A 138		48.124	3.761	15.523		22.14	Ą
	ATOM	547	CG		A 138		47.432	2.448	15.201	1.00	24.90	A
5	MOTA	548	OD1	ASP A	A 138		46.631	2.423	14.241	1.00	24.78	A
	MOTA	549	OD2	ASP A	A 138		47.691	1.443	15.897		25.39	A
	ATOM	550	С		A 138		46.031	4.991	16.138		20.47	
	ATOM	551	Ö	ASP A			45.967					A
								4.248	17.118		19.06	A
	ATOM	552	N		A 139		45.075	5.852	15.810		18.27	A
10	ATOM	553	CA	HIS A	139		43.869	6.016	16.606	1.00	18.21	A
	ATOM	554	CB	HIS A	139		44.096	7.157	17.612	1.00	15.84	A
	ATOM	555	CG	HIS A			42.985	7.332	18.600		15.24	A
	ATOM	556		HIS A			42.884	6.964	19.900		13.97	A
	ATOM	557		HIS A								
1.5							41.791	7.943	18.280		14.74	A
15	ATOM	558		HIS A			41.002	7.944	19.341		14.19	. А
	ATOM	559	NE2	HIS A	139		41.641	7.356	20.336	1.00	14.15	A
	ATOM	560	С	HIS A	139		42.715	6.330	15.654	1.00	18.50	· A
	ATOM	561	0	HIS A	139		42.879	7.080	14.693		20.80	A
	ATOM	562	N	PRO A	140		41.527	5.767	15.913		18.32	A
20	ATOM	563	CD	PRO A			41.143	4.984	17.100		16.71	A
20												
		00.	CA	PRO F			40.367	6.001	15.048		17.43	Α
	MOTA	565	CB	PRO I			39.273	5.157	15.704		16.64	A
	ATOM	566	CG	PRO A	140		39.643	5.204	17.152		18.43	A
	ATOM	567	С	PRO F	140		39.914	.7.441	14.803	1.00	18.77	Α
25	ATOM	568	0	PRO P	140		39.207	7.695	13.831	1.00	19.88	A
	ATOM	569	N	PHE A			40.301	8.381	15.664		17.14	A
	ATOM	570	CA	PHE A			39.874	9.767	15.477		16.42	. A
				PHE A								
	ATOM.	571	CB				39.568	10.422	16.836		14.60	A
	MOTA	572	$CG_{\mathbb{J}}$	PHE F			38.386	9.817	17.556		15.26	A
30	ATOM	573		PHE F			37.335	9.234	16.842	1.00	14.78	A
	ATOM	574	CD2	PHE A	141		38.297	9.880	18.942	1.00	13.70	A
	ATOM	575	CE1	PHE P	141		36.215	8.727	17.502	1.00	16.94	Α
	ATOM	576	CE2	PHE F	141		37.178	9.375	19.615	1.00	15.75	A
	ATOM	577	CZ	PHE F			36.135	8.799	18.893		16.89	A
35	ATOM	578	C	PHE F			40.857	10.641	14.694		16.15	A
55												
	ATOM	579	0	PHE F			40.799	11.871	14.761		17.35	A
	ATOM	580	N	PHE P			41.748	10.011	13.941		15.88	. A
	ATOM	581	ca	PHE A	142		42.727	10.756	13.154	1.00	17.89	A
	MOTA	582	CB	PHE P	142		44.115	10.645	13.793	1.00	17.57	A
40	ATOM	583	CG	PHE A	142		44.240	11.371	15.103	1.00	18.74	А
	ATOM	584	CD1	PHE A	142		44.559	12.726	15.135		17.77	A
	MOTA	585		PHE A			43.997	10.711	16.304		18.74	A
	ATOM	586		PHE A			44.632		16.347		15.77	A
								13.417				
	ATOM	587		PHE A			44.065	11.393	17.522		17.56	A
45	ATOM	588	cz	PHE A			44.383	12.747	17.542		17.14	A
	MOTA	589	С	PHE A	142		42.793	10.231	11.729	1.00	19.12	A
	ATOM	590	0	PHE A	142		42.659	9.030	11.504	1.00	20.01	A
	ATOM	591	N	VAL A	143		42.978	11.135	10.769	1.00	18.72	А
	ATOM	592	CA	VAL A			43.102	10.735	9.371		18.52	A
50	ATOM	593	CB	VAL A			43.294	11.961	8.440		20.66	A
50				VAL A								
	ATOM	594	_				43.843	11.521	7.080		21.29	A
	ATOM	595	CG2	VAL A			41.958	12.673	8.252		22.97	A
	ATOM	596	С	VAL A	. 143		44.342	9.865	9.330	1.00	18.68	A
	ATOM	597	0	VAL A	143		45.355	10.199	9.943	1.00	18.42	A
55	MOTA	598	N	LYS A			44.259	8.745	8.623	1.00	18.30	А
	ATOM	599	CA	LYS A			45.384	7.824	8.535		18.78	A
	ATOM	600	CB	LYS A			44.889	6.373	8.608		22.27	· A
	ATOM	601	CG	LYS A			46.017	5.340	8.557		29.72	A
	ATOM	602	CD	LYS A	. 144	,	45.491	3.912	8.674	T.00	34.16	·A

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	MOTA	603	CE LYS A 144	46	.631	2.896	8.577	1.00	37.67		A
•	MOTA	604	NZ LYS A 144	46	.138	1.484	8.629	1.00	39.02		A
	ATOM	605	C LYS A 144	46	.192	8.002	7.261	1.00	18.53		Α
	ATOM	606	O 'LYS A 144	4.5	. 643	8.314	6.200	1.00	18.18		Α
5	ATOM	607	N LEU A 145	47	.502	7.816	7.385	1.00	16.79		A
_	ATOM	608	CA LEU A 145			7.900	6.251	1.00			A
	ATOM	609	CB LEU 145			8.653	6.641	0.50			AC1
	ATOM	610	CG LEU 145			8.902	5.549	0.50			AC1
	ATOM	611	CD1 LEU 145	-		9.799	6.093	0.50			AC1
10		612	CD2 LEU 145			7.581	5.069	0.50			AC1
10	MOTA	613	C LEU A 145			6.450	5.907	1.00			A
	MOTA	614	O LEU A 145			5.772	6.659	1.00			Α
	ATOM					5.972	4.782	1.00			A
	ATOM	615				4.593	4.358	1.00			Α
	MOTA	616				4.098	3.486	1.00			A
15	ATOM	617	CB TYR A 146			3.926	4.214	1.00			A
	ATOM	618	CG TYR A 146			4.995	4.377	1.00			A
	ATOM	619	CD1 TYR A 146				5.039	1.00			A
	MOTA	620	CE1 TYR A 146			4.827	4.735	1.00			A
	ATOM	621	CD2 TYR A 146			2.686		1.00			A
20	ATOM	622	CE2 TYR A 146			2.506	5.399				A
	MOTA	623	CZ TYR A 146			3.576	5.544	1.00			A
	MOTA	624	OH TYR A 146			3.376	6.169	1.00		•	A
	MOTA	625	C TYR A 146			4.376	3.582				A
	MOTA	626	O TYR A 146			3.338	3.715	1.00			A
25	MOTA	627	N PHE A 147			5.350	2.765		18.09		
	ATOM	628	CA PHE A 147			5.203	1.952	1.00			A
	ATOM	629	CB PHE A 147			4.258	0.783	1.00			A
	ATOM	630	CG PHE A 147			4.699	-0.070	1.00			A
	ATOM	631	CD1 PHE A 147		.967	5.752	-0.975	1.00			A
30	ATOM	632	CD2 PHE A 147			4.075	0.053	1.00			A
	ATOM	633	CE1 PHE A 147		.886	6.178	-1.742		19.62		A
	MOTA	634	CE2 PHE A 147		.503	4.492	-0.710	-	18.56		A
	MOTA	635	CZ PHE A 147		.647	5.546	-1.610		19.27		A
	ATOM	636	C PHE A 147		.768	6.533	1.395		17.13		A
35	MOTA	637	O PHE A 147		.045	7.528	1.452		14.43.		A
	ATOM	638	N THR A 148		.981	6.534	0.854		17.12		A
	ATOM	639	CA THR A 148		.541	7.718	0.232		17.96		A
	ATOM	640	CB THR A 148		.449	8.531	1.197		21.51		A
	ATOM	641	OG1 THR A 148		.605	7.760	1.537		18.83		A
40	ATOM	642	CG2 THR A 148		.700	8.897	2.472		19.60		A
	ATOM	643	C THR A 148		.386	7.262	-0.946		20.31		A
	MOTA	644	O THR A 148		.860	6.124	-0.991		18.94		A
	ATOM	645	N PHE A 149		.543	8.149	-1.916		19.16		A
	ATOM	646	CA PHE A 149		.368	7.877	-3.073		18.01		A
45	ATOM	647	CB PHE A 149		.748	6.801	-3.989		17.23		A
	ATOM	648	CG PHE A 149	53	.389	7.144	-4.544		16.88		A
	ATOM	649	CD1 PHE A 149	53	.262	7.888	-5.712		18.58		A
	MOTA	650	CD2 PHE A 149		.235	6.668	-3.927		17.31		A
	MOTA	651	CE1 PHE A 149	52	.007	8.149	-6.267		19.26		A
50	ATOM	652	CE2 PHE A 149	50	.972	6.923	-4.470		19.17		A.
	MOTA	653	CZ PHE A 149	50	.858	7.663	-5.642		19.60		A
	ATOM	654	C PHE A 149	55	.542	9.205	-3.774		20.85		A
	ATOM	655	O PHE A 149	54	.934	0.200	-3.376		19.76		A
•	ATOM	656	N GLN A 150	56	398	9.241	-4.782		19.79		A
55	ATOM	657	CA GLN A 150	56	6.636	10.481	-5.497		24.03		A
- •	ATOM	658	CB GLN A 150	.57	.659 1	1.347	-4.739		24.45		A
	ATOM	659	CG GLN A 150	58	.986	10.645	-4.414		26.28		A
	ATOM	660	CD GLN A 150			L1.558	-3.692		29.02		A
	ATOM	661	OE1 GLN A 150	60	.693	12.353	-4.321	1.00	27.05		A
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	ATOM.	662	NE2	GLN A	150		60.042	11.449	-2.365	1.00	26.47	Α
	ATOM	663	С	GLN A			57.160	10.203	-6.885	1.00	23.88	A
	ATOM	664	Ō	GLN A	150		57.673	9.118	-7.158	1.00	24.79	A
	ATOM	665	N	ASP A			56.987	11.171	-7.774	1.00		- A
5	ATOM	666	CA	ASP A			57.527	11.047	-9.117	1.00	26.49	A
•	ATOM	667	CB	ASP A			56.437		-10.199	1.00	24.54	A
	ATOM	668	CG	ASP A			55.544		-10.064		24.95	A
	ATOM	669		ASP A			56.005	13.379	-9.561		22.44	A
	ATOM	670		ASP A			54.369		-10.490		25.72	A
10	ATOM	671	C	ASP A			58.515	12.203	-9.220		28.63	A
10	ATOM	672	0	ASP A			58.890	12.780	-8.194		27.83	A
	ATOM	673	N	ASP A			58.934		-10.426		29.21	Α.
		674	CA	ASP A			59.907		-10.562		31.88	A
	ATOM	675	CB	ASP A			60.325		-12.026		33.94	A
16	MOTA			ASP I			61.033		-12.557		38.88	A
15	ATOM	676	CG	ASP A			61.817		-11.791		39.67	A
	ATOM	677		ASP A			60.817		-13.738		41.57	A
	ATOM	678		ASP A			59.487		-10.013		30.90	A
	ATOM	679	C	ASP A			60.316	15.735	-9.482		31.69	A
20	MOTA	680	0	GLU A			58.207		-10.107		29.44	A
20	MOTA	681	N	GLU A			57.767	16.632	-9.646		28.69	A
	ATOM	682	CA	GLU A			56.984		-10.766		32.90	A
	MOTA	683	CB	GLU A			57.451		-12.183		40.57	A
	ATOM	684	CG	GLU A			56.920		-12.675		45.78	A
25	ATOM	685	CD	GLU A			55.682		-12.760		48.91	A
25	MOTA	686		GLU Z			57.736		-12.979		48.95	A
	MOTA	687		GLU A			56.929	16.683	-8.372		26.43	A
	MOTA	688	C		1 153 1 153		56.947	17.688	-7.660		25.08	A
	ATOM	689	0		1 153	•	56.205	15.610	-8.069		22.39	A
20	ATOM .	690	N CA	LYS A			55.318	15.631	-6.912		21.43	· A
30	ATOM	691 692	CB	LYS A			53.861	15.628	-7.398		20.33	A
	ATOM ATOM	693	CG		1 154		53.505	16.716	-8.403		21.92	A
	ATOM	694	·CD		A 154		52.211	16.375	-9.146		19.70	Α
		695	CE	LYS A			51.775		-10.077		20.04	A
35	ATOM ATOM	696	NZ		1 154		50.631		-10.951		19.97	A
33		697	C		A 154	,	55.458	14.522	-5.881		20.43	Α
	ATOM ATOM	698	0		A 154		55.949	13.426	-6.173		21.13	Α
	ATOM	699	N		1 155 1 155		54.985	14.832	-4.676		19.69	Α
	ATOM	700	CA		A 155		54.950	13.900	-3.553		19.10	Α
40 -	ATOM	701	CB		A 155		55.362	14.588	-2.252	1.00	19.65	Α
70	ATOM	702	CG		A 155		56.740	15.234	-2.129	1.00	21.20	A
	ATOM	702		LEU Z			56.848	15.918	-0.770	1.00	23.42	A
	ATOM	703		LEU Z			57.816	14.174	-2.277		23.08	A
	ATOM	705	C		A 155		53.478	13.507	-3.427	1.00	18.87	A
45	ATOM	705	Ö		A 155		52.600	14.348	-3.620		18.61	A
43	ATOM	707	N		A 156		53.209	12.249	-3.091		15.02	A
	ATOM	708	CA		A 156		51.834	11.783	-2.934		16.29	A
	ATOM	709	CB		A 156		51.470	10.769	-4.029		14.20	A
	ATOM	710	CG		A 156		51.603	11.273	-5.449		17.29	A
50	ATOM	711	CD1				52.857	11.429	-6.045		16.46	A
50	ATOM	712	CE1		A 156		52.978	11.884	-7.360		18.68	A
		713		TYR			50.474	11.588	-6.202	1.00	16.43	A
	ATOM ATOM	713		TYR .			50.583	12.048	-7.512		16.31	Α
	ATOM	715	CZ		A 156		51.835	12.192	-8.083		18.17	A
55	ATOM	716	OH		A 156		51.941	12.651	-9.371		17.47	A
,,	ATOM	717	C		A 156		51.657	11.108	-1.572		16.32	A
	ATOM	718	Ö		A 156		52.412	10.197	-1.235		16.27	. А
	ATOM	719	N		A 157		50.678	11.568	-0.792		15.47	A
	ATOM	720	CA		A 157		50.385	10.966	0.508		16.66	A
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	MOTA	721	СВ	PHE	À	157		50.324	12.014	1.629	1.00	16.91		A
	ATOM	722	CG	PHE	Α	157		51.631	12.708	1.907		18.96		Ä
	MOTA	723	CD1	PHE	Α	157		52.821	12.261	1.340		20.31		A
	ATOM	724	CD2	PHE	Α	157		51.664	13.829	2.732		21.12		A
5	ATOM	725	CE1	PHE	Α	157		54.025	12.926	1.585		22.08		A
	ATOM	726	CE2	PHE	Α	157		52.865	14.500	2.982		22.18		A.
	ATOM	727	CZ	PHE	Α	157		54.045	14.045	2.405		21.27		A.
	ATOM	728	С			157		49.016	10.308	0.404		16.52		A
	ATOM	729	0			157		48.029	10.979	0.110		17.32		A
10	ATOM	730	N			158		48.953	9.002	0.644		15.97		A
	ATOM	731	CA			158		47.684	8.299	0.572		16.13		A
	ATOM	732	C			158		47.000	8.383	1.920		14.94		A
	ATOM	733	0			158		47.445	7.756	2.879		16.28		A
	ATOM	734	N	-		159		45915	9.145	1.989		13.50		A
15	ATOM	735	CA			159		45.191	9.340	3.241		15.20		A.
.*3	ATOM	736	CB			159		45.031	10.835	3.517		14.20	· 7	
	ATOM	737				159		46.270	11.726	3.385		19.00		
	ATOM	738		LEU				45.847	13.188	3.477		17.12		-1. A
	ATOM	739		LEU				47.275	11.390	4.471		14.71		
20	ATOM	740	C			159		43.809	8.716	3.232		15.53	I	
20	ATOM	741	Ö			159		43.232	8.472	2.177		16.05		A.
	ATOM	742	N			160		43.268	8.469	4.418		15.86	I	
	ATOM	743	CA			160		41.932	7.917	4.498		19.01	7	
	ATOM	744	CB			160		41.566	7.582	5.949		22.90		
25	ATOM	745	OG			160		41.901	8.629	6.833		24.18		
23	ATOM	746	C			160		40.987	8.968	3.924		20.43	I	
	ATOM	747	Ö			160		41.213	10.173	4.062		19.96	Į	
	ATOM	748	N			161		39.945	8.508	3.250		19.20	Į	
	ATOM	749	CA			161		38.975	9.406	2.644		20.37	I	
30	ATOM	750	CB			161		38.471	8.785	1.332		20.00	Į	
50	ATOM	751	CG			161		37.314	9.502	0.666		20.72	Į	
	ATOM	752	CD1					37.222	10.895	0.682		18.22	Ī	
	ATOM	753		TYR				36.180	11.557	0.029		22.24	Į	
	ATOM	754	CD2					36.333	8.784	-0.020		20.53	Į	
35	ATOM	755	CE2					35.287	9.436	-0.678		24.24	F	
	ATOM	756	CZ	TYR				35.218	10.822	-0.648		22.32	F	
	ATOM	757	OH	TYR				34.194	11.471	-1.298		23.03	P	
	ATOM	758	C	TYR				37.812	9.681	3.598		20.14	- P	
	ATOM	759	Õ	TYR				36.959	8.819	3.810		19.53		
40	ATOM	760	N	ALA				37.791	10.880	4.178		19.92	P	
. •	ATOM	761	CA	ALA				36.721	11.271			21.07	P	
	ATOM	762	CB	ALA				37.187	12.419	6.002		19.60	P	
	ATOM	763	C	ALA				35.542	11.712	4.238		22.07	P	
	ATOM	764	Ö	ALA				35.436	12.875	3.860		20.66	P	
45	ATOM	765	N	LYS				34.653	10.769	3.945		23.27	P	
	ATOM	766	CA	LYS				33.503	11.017	3.080		27.12	P	
	ATOM	767	CB	LYS				32.663	9.741	2.963		29.68	7	
	ATOM	768	CG	LYS				33.455	8.524	2.515		37.67	P	
	ATOM	769	CD	LYS				32.556	7.310	2.321		42.24	P	
50	ATOM	770	CE	LYS				33.373	6.034	2.185		44.48	Z	
	ATOM	771	NZ	LYS				34.143	5.735	3.430		44.88	P	
	ATOM	772	C	LYS				32.581	12.186	3.411		25.78	. A	
	ATOM	773	0	LYS				32.103	12.863	2.506		26.53	A	
	ATOM	774	N	ASN				32.327	12.441	4.689		24.57	Æ	
55	ATOM	775	CA	ASN				31.420	13.522	5.033		23.77	A	
	ATOM	776	CB	ASN				30.610	13.129	6.265		25.02	<i>2</i> A	
	ATOM	777	CG	ASN				29.537	12.101	5.932		27.54	A	
	ATOM	778		ASN				28.772	12.281	4.983		28.79	A	
	ATOM	779		ASN				29.475	11.024	6.704		27.13	A	
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	ATOM	780	С	ASN	Α	164	31.999	14.931	5.169	1.00	24.43	A
	ATOM	781	0	ASN	Α	164	31.306	15.856	5.589	1.00	23.98	·A
	ATOM	782	N	GLY	Α	165	33.262	15.097	4.795	1.00	21.56	A
	ATOM	783	CA	GLY	A.	165	33.873	16.414	4.836	1.00	24.39	A
5	ATOM	784	C	GLY	Α	165	34.191	17.043	6.181	1.00	23.62	A
	ATOM	785	0	GLY	Α	165	34.380	16.352	7.177	1.00	23.26	A
	ATOM	786	N	GLU	Α	166	34.234	18.373	6.186	1.00	23.22	A
	ATOM	787	CA	GLU	Α	166	34.563	19.176	7.362	1.00	24.54	Α
	ATOM	788	CB	GLU	Α	166	35.055	20.558	6.913	1.00	25.04	A
10	ATOM	789	CG	GLU	Α	166	36.419	20.569	6.229	1.00	26.48	Α
	ATOM	790	CD	GLU	Α	166	36.699	21.889	5.517	1.00	30.02	Α
	ATOM	791	OE1	GLU	A	166	36.081	22.906	5.889	1.00	29.33	Α
	ATOM	792	OE2	GLU	Α	166	37.544	21.916	4.596	1.00	30.48	A
	ATOM	793	С	GLU	Α	166	33.436	19.372	8.369	1.00	24.44	Α
15	ATOM	794	0	GLU	A	166	32.279	19.541	8.001	1.00	22.76	A
	ATOM	795	N	LEU	Α	167	33.791	19.370	9.649	1.00	22.95	Α
	MOTA	796	CA	LEU	Α	167	32.813	19.581	10.707	1.00	22.26	A
	ATOM	797	CB	LEU	Α	167	33.497	19.481	12.073	1.00	22.32	A
	ATOM	798	CG	LEU	Α	167	32.706	19.923	13.306	1.00	22.04	A
20	ATOM	799	CD1	LEU	Α	167	31.454	19.074	13.463	1.00	19.66	Α
	ATOM	800	CD2	LEU	A	167	33.597	19.805	14.537	1.00	21.17	A
	MOTA	801	С	LEU	Α	167	32.193	20.971	10.529	1.00	23.49	A
	ATOM	802	0	LEU	Α	167	31.047	21.209	10.907	1.00	23.56	A
	ATOM	803	N	LEU	Α	168	32.960	21.887	9.948	1.00	24.25	А
25	ATOM	804	CA	LEU	A	168	32.473	23.245	9.722	1.00	26.64	A
	ATOM	805	CB	LEU	Α	168	33.560	24.099	9.066	1.00	25.62	A
	ATOM	806	CG	LEU	Α	168	33.198	25.546	8.707	1.00	27.34	Α
	ATOM	807	CD1	LEU	А	168	32.718	26.296	9.946	1.00	26.42	Α
	ATOM	808	CD2	LEU	Α	168	34.418	26.238	8.119	1.00	26.74	Α
30	ATOM	809	С	LEU	A	168	31.234	23,218	8.829	1.00	27.13	A
	ATOM	810	Ο.	LEU	Α	168	30.297	23.989	9.030	1.00	26.01	A
	ATOM	811	N	LYS	Α	169	31.233	22.320	7.848	1.00	26.41	A
	ATOM	812	CA	LYS	Α	169	30.106	22.210	6.934	1.00	27.70	Α
	ATOM	813	СВ	LYS	Α	169	30.324	21.064	5.945	1.00	30.49	Α
35	ATOM	814	CG	LYS	A	169	29.151	20.854	4.993	1.00	32.47	Α
	ATOM	815	CD	LYS	Α	169	29.407	19.728	3.998	1.00	35.98	Α
	ATOM	816	CE	LYS	Α	169	29.462	18.372	4.683	1.00	38.53	Α
	ATOM	817	NZ	LYS	Α	169	29.622	17.263	3.702	1.00	41.00	A
	ATOM	818	С	LYS	Α	169	28.801	21.985	7.682	1.00	28.12	Α
40	ATOM	819	0	LYS	Α	169	27.785	22.608	7.371	1.00	28.08	A
	ATOM	820	N	TYR	A	170	28.826	21.094	8.668	1.00	26.53	A
	ATOM	821	CA	TYR	А	170	27.624	20.791	9.434	1.00	26.95	A
	ATOM	822	CB	TYR	A.	170	27.810	19.476	10.193		25.03	Α
	ATOM.	823	CG	TYR	Α	170	27.898	18.300	9.251	1.00	26.65	A
45	ATOM	824	CD1	TYR	Α	170	26.745	17.661	8.790		28.27	Α
	ATOM	825	CE1	TYR	Α	170	26.814	16.642	7.839		26.85	A
	ATOM	826	CD2	TYR	A	170	29.127	17.884	8.742		27.83	A
	ATOM	827	CE2	TYR	Α	170	29.209	16.869	7.792		27.19	A
	ATOM	828	CZ	TYR	Α	170	28.049	16.254	7.343		30.02	A
50	ATOM	829	ОН	TYR	Α	170	28.130	15.268	6.382		29.23	A
	ATOM	830	С	TYR	A	170	27.229	21.918	10.376		27.59	A
	ATOM	831	0	TYR	Α	170	26.045	22.122	10.642		29.25	A
	ATOM	832	N	ILE	A	171	28.208	22.660	10.882		28.16	A
	ATOM	833	CA,	ILE	A	171	27.883	23.770	11.763		29.03	A
55	ATOM	834	CB	ILE	A	171	29.151	24.435	12.337		27.51	A
	ATOM	835		ILE			28.773	25.705	13.084		27.97	A
	ATOM	836	CG1	ILE	A	171	29.872	23.458	13.272		26.70	A
	ATOM	837		ILE			31.163	23.996	13.856		24.07	A
	ATOM	838	С	ILE	A	171	27.094	24.796	10.944	1.00	31.41	Α

	ATOM	839	0	TIF	A 171		26.088	25.335	11.407	1.00 31.69	. A
	ATOM	840	N		A 172	•	27.546	25.047	9.719	1.00 33.21	A
					A 172		26.874	26.000	8.844	1.00 36.54	A
	MOTA	841	CA						7.616	1.00 30.34	A.
_	MOTA	842	CB		A 172		27.734	26.314			
5	ATOM	843	CG		A 172		29.057	27.011	7.912	1.00 41.65	A
	ATOM	844	CD		A 172		29.708	27.492	6.616	1.00 45.29	A
	MOTA	845	NE		A 172		31.037	28.070	6.812	1.00 48.51	A
	ATOM	846	CZ		A 172		31.314	29.059	7.658	1.00 51.53	A
	ATOM	847	NH1	ARG	A 172		30.355	29.593	8.406	1.00 53.75	A
10	ATOM	848	NH2	ARG	A 172		32.553	29.526	7.748	1.00 51.21	A
	ATOM	849	С	ARG	A 172		25.528	25.459	8.378	1.00 37.67	A
	ATOM	850	0	ARG	A 172		24.550	26.200	8.288	1.00 39.09	A
	ATOM	851	N	LYS	A 173		25.481	24.163	8.092	1.00 38.44	Α
	ATOM	852	CA	LYS	A 173		24.259	23.528	7.619	1.00 39.25	Α
15	ATOM	853			A 173		24.523	22.061	7.272	1.00 41.89	A
20	ATOM	854	CG		A 173		23.279	21.298	6.830	1.00 45.52	Α.
	ATOM	855	CD		A 173		23.557	19.808	6.653	1.00 49.60	Α
	ATOM	856	CE		A 173		24.477	19.530	5.469	1.00 52.63	A
		857	NZ		A 173		23.855	19.894	4.160	1.00 54.61	A
20	ATOM	858	C		A 173		23.033	23.608	8.595	1.00 39.30	A
20	ATOM						21.981	23.960	8.201	1.00 39.62	A
	ATOM	859	0		A 173		23.320	23.282	9.863	1.00 37.96	A
	MOTA	860	N		A 174			23.202	10.833	1.00 37.36	A
	ATOM	861	CA		A 174		22.229		11.652	1.00 37.44	A
	ATOM	862	CB		A 174		22.159	21.998		1.00 37.44	A
25	MOTA	863			A 174		22.058	20.802	10.709	1.00 38.37	A
	ATOM	864			A 174		23.397	21.850	12.532		A A
	MOTA	865			A 174		23.355	20.620	13.418	1.00 36.85	
	ATOM	866	С		A 174		22.259	24.492	11.801	1.00 36.71	A
	MOTA	867	0		A 174		21.448	24.556	12.724	1.00 38.05	A
30	ATOM	868	N	GLY	A 175		23.185	25.423	11.592	1.00 35.48	A
	ATOM	869	CA	GLY	A 175		23.265	26.585	12.462	1.00 35.29	A
	ATOM	870	С	GLY	A 175		24.053	26.360	13.737	1.00 35.06	A
	ATOM	871	0	GLY	A 175		25.066	27.019	13.970	1.00 37.46	A
	ATOM	872	N		A 176		23.581	25.441	14.571	1.00 33.94	A
35	ATOM	873	CA	SER	A 176		24.253	25.113	15.822	1.00 32.84	A
	ATOM	874	СВ	SER	A 176		23.938	26.155	16.901	1.00 33.54	A
	ATOM	875	OG		A 176		22.599	26.056	17.347	1.00 34.86	A
	ATOM	876	C		A 176		23.796	23.731	16.276	1.00 32.34	A
	ATOM	877	ō		A 176		22.726	23.263	15.884	1.00 32.82	A
40	ATOM	878	N		A 177		24.609	23.085	17.103	1.00 29.39	Α
40	ATOM	879	CA		A 177		24.313	21.743	17.597	1.00 27.20	A
	ATOM	880	CB		A 177		25.621	20.989	17.865	1.00 26.39	A
	ATOM	881	CG		A 177		26.372	20.585	16.622	1.00 26.18	A
		882			A 177		26.210	21.277	15.426	1.00 25.30	Α
45	ATOM				A 177		27 266		16.662		A
45	ATOM	883					26.923	20.912	14.290	1.00 26.59	A
	ATOM	884			A 177		27.986	19.143	15.532	1.00 26.06	A
	ATOM	885			A 177			19.841	14.343	1.00 25.42	A
	ATOM	886	CZ		A 177		27.815	21.752	18.884	1.00 27.00	A
	MOTA	887	C.		A 177		23.500		19.747	1.00 26.48	A
50	MOTA	888	0		A 177		23.704	22.610		1.00 26.70	A
	ATOM	889	N		A 178		22.578	20.802	19.022	1.00 26.70	A
	ATOM	890	CA		A 178		21.816	20.729	20.260		
	ATOM	891	CB		A 178		20.621	19.773	20.142	1.00 29.90	A
	MOTA	892	CG		A 178		21.020	18.372	19.720	1.00 32.28	A
55	ATOM	893			A 178		22.157	17.949	20.014	1.00 35.21	A
	ATOM	894	OD2	ASP	A 178	}	20.179	17.683	19.105	1.00 34.79	A
	MOTA	895	С	ASP	A 178	}	22.810	20.228	21.311	1.00 25.03	A
	ATOM	896	0		A 178		23.974	19.968	20.992	1.00 21.24	A
	ATOM	897			A 179		22.361	20.083	22.552	1.00 23.60	A

	ATOM	898	CA	GLU A	179	23.247	19.644	23.619	1.00 25.18	A
	ATOM	899	СВ	GLU A		22.542	19.770	24.971	1.00 27.60	A
	ATOM	900	CG	GLU A	179	23.324	19.176	26.130	1.00 32.58	A
	ATOM	901	CD	GLU A	179	22.997	19.845	27.449	1.00 35.82	A
5	ATOM	902	-			21.825	20.224	27.645	1.00 35.95	· A
•	ATOM.	903		GLU A		23.912	19.984	28.291	1.00 38.19	A
	ATOM	904	C	GLU A		23.808	18.235	23.450	1.00 24.08	. A
	ATOM	905	Ö	GLU A		24.977	17.989	23.756	1.00 22.79	A
	ATOM	906	N	THR A		22.983	17.316	22.961	1.00 23.36	A
10		907	CA	THR A		23.412	15.935	22.761	1.00 22.15	A
10	MOTA		CB	THR A		22.224	15.054	22.320	1.00 23.77	A
	ATOM	908		THR A		21.222	15.075	23.341	1.00 26.37	A
	ATOM	909		THR A		22.670	13.616	22.088	1.00 22.66	A
	ATOM	910		THR A		24.533	15.830	21.724	1.00 22.01	A
	ATOM	911	C	THR A		25.533	15.141	21.944	1.00 19.87	A
15	ATOM	912	0	CYS A		24.365	16.511	20.596	1.00 21.21	A
	MOTA	913	N			25.372	16.480	19.541	1.00 22.22	A
	ATOM	914	CA	CYS A		24.800	17.065	18.250	1.00 24.62	A
	ATOM	915	CB	CYS A			16.080	17.560	1.00 29.50	A
	ATOM	916	SG	CYS A		23.435 26.633	17.232	19.954	1.00 23.07	A
20	ATOM	917	C	CYS A				19.608	1.00 23.07	A
	ATOM	918	0	CYS A		27.746	16.827		1.00 23.33	A
	ATOM	919	N	THR A		26.463	18.325	20.695 21.161	1.00 22.70	A
	ATOM	920	CA	THR A		27.606	19.103		1.00 21.43	A
	ATOM	921	CB	THR A		27.167	20.346	21.978	1.00 22.50	A
25 .	ATOM	922	OG1			26.459	21.262	21.134 22.565	1.00 22.30	A
	MOTA	923	CG2	THR A		28.379	21.046		1.00 18.30	A
	ATOM	924	С	THR A		28.454	18.215	22.071	1.00 21.40	A
	MOTA	925	0	THR A		29.669	18.090	21.894	1.00 19.93	A
	ATOM	926	N	ARG A		27.798	17.602	23.050	1.00 18.37	A
30	MOTA	927	CA	ARG A		28.468	16.723	23.996		AC1
	MOTA	928	CB	ARG	183	27.455	16.140	24.984		AC1
	ATOM	929	CG	ARG	183	28.030	15.062	25.887	0.50 18.77 0.50 21.19	AC1
	MOTA	930	CD	ARG	183	27.021	14.571	26.925		ACÍ
	MOTA	931	NE	ARG	183	26.605	15.642	27.824	0.50 19.46 0.50 20.45	AC1
35	MOTA	932	CZ	ARG	183	25.496	16.362	27.679		AC1
	ATOM	933		ARG	183	24.672	16.123	26.666	0.50 19.81	AC1
	MOTA	934	NH2	ARG	183	25.224	17.338	28.539	0.50 17.11 1.00 20.02	ACI
	MOTA	935	С	ARG A		29.206	15.577	23.302	1.00 20.02	A
	MOTA	936	Ο.	ARG A		30.383	15.333	23.573		A
40	MOTA	937	N	PHE A		28.520	14.871	22.409	1.00 19.24	A
	MOTA	938	CA	PHE A		29.144	13.746	21.722	1.00 18.04	, A
	MOTA	939	CB	PHE A		28.158	13.078	20.764	1.00 21.05	A
	MOTA	940	CG	PHE A		28.719	11.857	20.098	1.00 22.67	
	MOTA	941	CD1	PHE A		28.717	10.630	20.754	1.00 22.97	A
45	MOTA	942		PHE A		29.317	11.949	18.850	1.00 19.97	A
	MOTA	943		PHE A		29.308	9.510	20.176	1.00 23.53	A
	ATOM	944	CE2	PHE A		29.915	10.833	18.263	1.00 24.11	A
	ATOM	945	cz	PHE A	184	29.910	9.613	18.928	1.00 22.97	, A
	ATOM	946	С	PHE A	184	30.403	14.127	20.941	1.00 17.99	Α.
50	ATOM	947	0	PHE A	184	31.461	13.531	21.130	1.00 18.89	A
	MOTA	948	N	TYR A		30.292	15.110	20.056	1.00 15.73	A
	ATOM	949	CA	TYR A	185	31.443	15.519	19.265	1.00 15.72	A
	ATOM	950	CB	TYR A	185	30.992	16.413	18.111	1.00 17.33	A
	ATOM	951	CG	TYR A		30.364	15.584	17.015	1.00 19.37	A
55	ATOM	952	CD1	TYR A	185	31.159	14.809	16.168	1.00 16.53	A
	ATOM	953		TYR A		30.590	13.952	15.232	1.00 18.12	A
	ATOM	954		TYR A		28.976	15.484	16.892	1.00 18.18	A
	ATOM	955		TYR A		28.398	14.623	15.956	1.00 18.90	A
	ATOM	956	CZ	TYR A		29.211	13.861	15.133	1.00 18.41	A
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	ATOM	957	ОН	TYR .	A 185		28.650	12.995	14.218	1.00 20.	48 A
	ATOM	958	С	TYR .	A 185		32.544	16.172	20.083	1.00 15.	79 A
	ATOM	959	0		A 185		33.720	16.015	19.766	1.00 17.	69 A
	ATOM	960	N	THR .	A 186		32.176	16.887	21.142	1.00 15.	
5	ATOM	961	CA		A 186		33.184	17.504	21.997	1.00 16.	
_	ATOM	962	CB		A 186		32.559	18.403	23.094	1.00 16.	
	ATOM	963	OG1		A 186		31.866	19.503	22.481	1.00 14.	
	ATOM	964	CG2	•	A 186		33.656	18.953	24.019	1.00 14.	
•	ATOM	965	C		A 186		33.954	16.375	22.680	1.00 15.	
10	ATOM	966	Ö		A 186		35.176	16.443	22.823	1.00 13.	
10	ATOM	967	N		A 187	•	33.234	15.333	23.097	1.00 14.	
		968			A 187		33.869	14.196	23.757	1.00 14.	
	ATOM	969.	CA		A 187		32.810	13.195	24.224	1.00 14.	
	ATOM		CB		A 187		34.875	13.193	22.821	1.00 14.	
15	ATOM	970	C				35.972	13.136	23.247	1.00 14.	
15	ATOM	971	0		A 187				23.247		
	ATOM	972	N		A 188		34.516	13.340		1.00 14.	
	ATOM	973	CA		A 188		35.443	12.704	20.615	1.00 13.	
	ATOM	974	CB		A 188		34.782	12.449	19.251	1.00 12.	
	ATOM	975	CG		A 188		33.622	11.454	19.282	1.00 12.	
20	ATOM	976	CD		A 188		33.464	10.685	17.979	1.00 15.	
	MOTA	977			A 188		33.687	11.275	16.899	1.00 13.	
	ATOM	978			A 188		33.110	9.484	18.031	1.00 17.	
	MOTA	979	С		A 188		36.682	13.582	20.436	1.00 13.	
	MOTA	980	0		A 188		37.803	13.085	20.408	1.00 14.	
25	MOTA	981	N		A 189		36.486	14.893	20.326	1.00 13.	
	MOTA	982	CA		A 189		37.627	15.787	20.159	1.00 13.	••
	ATOM	983	СВ		A 189		37.169	17.247	19.939	1.00 13.	
	MOTA	984	CG2		A 189		38.381	18.165	19.822	1.00 12.	
	ATOM	985	CG1		A 189		36.302	17.332	18.671	1.00 13.	
30	MOTA	986			A 189		35.588	18.664	18.491	1.00 14.	
	MOTA	987	С	ILE .	A 189		38.530	15.702	21.394	1.00 14.	
	MOTA	988	0	ILE .	A 189		39.753	15.595	21.271	1.00 12.	
	MOTA	989	N	VAL .	A 190		37.927	15.751	22.582	1.00 14.	
	ATOM	990	CA		A 190		38.684	15.655	23.832	1.00 13.	
35	ATOM	991	CB	VAL .	A 190		37.743	15.690	25.061	1.00 14.	
	ATOM	992	CG1	VAL .	A 190		38.509	15.267	26.326	1.00 15.	
	ATOM	993	CG2	VAL .	A 190		37.160	17.082	25.233	1.00 12.	
	ATOM	994	С	VAL .	A 190		39.468	14.338	23.859	1.00 14.	
	ATOM	995	0	VAL .	A 190		40.634		24.250	1.00 13.	
40	MOTA	996	N		A 191		38.825	13.254	23.432	1.00 15.	
	ATOM	997	CA	SER .	A 191		39.478	11.943	23.421	1.00 16.	
	ATOM	998	CB	SER	191		38.470	10.857	23.041	0.50 16.	
	ATOM	999	OG	SER	191		39.018	9.569	23.238	0.50 16.	
	ATOM	1000	С	SER .	A 191		40.649	11.928	22.441	1.00 16.	
45	MOTA	1001	0		A 191		41.697	11.335	22.713	1.00 13.	
	ATOM	1002	N	ALA .	A 192		40.468	12.586	21.300	1.00 15.	
	ATOM	1003	CA	ALA .	A 192		41.518	12.645	20.292	1.00 14.	
	ATOM	1004	CB	ALA .	A 192		40.989	13.296	19.016	1.00 14.	
	ATOM	1005	С	ALA .	A 192		42.695	13.440	20.845	1.00 16.	
50	MOTA	1006	0		A 192		43.851	13.038	20.697	1.00 17.	
	ATOM	1007	N		A 193		42.401	14.563	21.496	1.00 15.	
	ATOM	1008	CA		A 193		43.459	15.392	22.067	1.00 15.	
	ATOM	1009	CB		A 193		42.884	16.712	22.600	1.00 12.	
	ATOM	1010	CG		A 193		42.445	17.721	21.525	1.00 15.	
55	ATOM	1011		LEU :	A 193		41.869	18.979	22.190	1.00 13.	97 A
	ATOM	1012			A 193		43.642	18.088	20.655	1.00 14.	58 A
	ATOM	1013	С		A 193		44.211	14.659	23.174	1.00 14.	49 A
	ATOM	1014		LEU .	A 193		45.427	14.813	23.310	1.00 16.	56 A
	ATOM	. 1015	N		A 194		43.500	13.870	23.975	1.00 13.	96 A

	ATOM	1016	CA	GLU A	194	44.179	13.123	25.032	1.00 14.08	Α
	ATOM	1017	CB	GLU A		43.190	12.295	25.857	1.00 14.65	· A
	ATOM	1018	CG	GLU A	194	43.882	11.301	26.789	1.00 17.09	Α
	MOTA	1019	CD	GLU A	194	42.924	10.592	27.730	1.00 19.59	А
5	ATOM	1020	OE1	GLU A	194	41.809	10.237	27.295	1.00 19.25	A
	ATOM	1021	OE2	GLU A	194	43.302	10.380	28.906	1.00 20.20	A
	MOTA	1022	С	GLU A		45.208	12.199	24.386	1.00 13.57	A
	MOTA	1023	0	GLU A		46.337	12.093	24.847	1.00 14.23	A
	ATOM	1024	N	TYR A		44.822	11.544	23.301	1.00 14.89	A
10	ATOM	1025	CA	TYR A		45.743	10.642	22.618	1.00 14.05	A
20	ATOM	1026	СВ	TYR A		45.030	9.910	21.488	1.00 10.30	Ā
	ATOM	1027	CG	TYR A		45.956	9.058	20.649	1.00 17.23	A
	ATOM	1028		TYR A		46.347	7.788	21.077	1.00 17.92	A
	ATOM	1029	CE1			47.203	6.996	20.304	1.00 17.30	A
15	MOTA	1030	CD2			46.445	9.524	19.428	1.00 19.77	
15	ATOM	1030		TYR A		47.299	8.744		1.00 18.51	. A
								18.650		A
	ATOM	1032	CZ	TYR A		47.671	7.481	19.094	1.00 20.24	A
	ATOM	1033	ОН	TYR A		48.506	6.705	18.325	1.00 21.89	A
20	ATOM	1034	C	TYR A		46.917	11.419	22.035	1.00 16.98	A
20	MOTA	1035	0	TYR A		48.081	11.047	22.203	1.00 14.61	A
	MOTA	1036	N	LEU A		46.599	12.507	21.347	1.00 16.30	A
	ATOM	1037	CA	LEU A		47.619	13.328	20.720	1.00 18.15	A
	MOTA	1038	CB	LEU A		46.969	14.502	19.982	1.00 18.59	A
	ATOM	1039	CG	LEU A		47.834	15.203	18.935	1.00 22.51	A
25	MOTA	1040		LEU A		48.222	14.206	17.841	1.00 20.94	A
	MOTA	1041		LEU A			16.375	18.338	1.00 22.98	A
	ATOM	1042	С	LEU A		48.592	13.844	21.763	1.00 17.75	A
	ATOM	1043	0	LEU A		49.801	13.644	21.649	1.00 18.33	A
	ATOM	1044	N	HIS A		48.064	14.495	22.792	1.00 17.12	A
30	MOTA	1045	CA	HIS A		48.913	15.042	23.842	1.00 18.47	A
,	MOTA	1046	CB	HIS A		48.069	15.866	24.817	1.00 15.90	A
	MOTA	1047	CG	HIS A		47.571	17.152	24.231	1.00 19.15	A
	ATOM	1048		HIS A		47.830	17.745	23.038	1.00 18.22	A
	ATOM	1049		HIS A		46.704	17.992	24.897	1.00 17.47	A
35	MOTA	1050		HIS A		46.450	19.047	24.139	1.00 19.74	A -
	ATOM	1051	NE2	HIS A		47.119	18.921	23.007	1.00 15.69	A
	MOTA	1052	С	HIS A		49.696	13.958	24.572	1.00 19.40	A
	ATOM	1053	0	HIS A		50.823	14.192	25.021	1.00 19.42	A
	MOTA	1054	N	GLY A		49.106	12.770	24.679	1.00 18.59	A
40	MOTA	1055	CA	GLY A		49.793	11.675	25.339		Α
	MOTA	1056	С	GLY A		51.075	11.307	24.612	1.00 21.86	Α
	ATOM	1057	0	GLY A		51.963	10.682	25.186	1.00 23.09	A
	ATOM	1058	N	LYS A		51.174	11.687	23.341	1.00 22.81	A
	ATOM	1059	CA	LYS A		52.368	11.401	22.549	1.00 24.43	A
45	MOTA	1060	CB	LYS A		51.990	10.905	21.154	1.00 26.00	A
	ATOM	1061	CG	LYS A		51.378	9.520	21.133	1.00 30.98	A
	MOTA	1062	CD	LYS A	199	51.291	9.002	19.708	1.00 36.85	A
•	MOTA	1063	CE	LYS A	199	50.832	7.559	19.682	1.00 40.37	Α
	MOTA	1064	NZ	LYS A	199	51.646	6.691	20.581	1.00 43.48	A
50	ATOM	1065	С	LYS A	199	53.253	12.631	22.414	1.00 23.88	A
	ATOM	1066	0	LYS A		54.144	12.669	21.568	1.00 24.97	A
	ATOM	1067	N	GLY A	200	52.997	13.638	23.243	1.00 24.00	A
	ATOM	1068	CA	GLY A		53.790	14.853	23.203	1.00 22.12	A
	ATOM	1069	С	GLY A	200	53.665	15.632	21.907	1.00 22.14	A
55	ATOM	1070	0	GLY A	200	54.632	16.231	21.439	1.00 22.41	A
	ATOM	1071	N	ILE A		52.475	15.630	21.320	1.00 20.00	A
	MOTA	1072	CA	ILE A		52.252	16.355	20.080	1.00 18.93	Α
	ATOM	1073	CB	ILE A	201	51.784	15.414	18.955	1.00 19.70	A
	ATOM	1074	CG2	ILE A	201	51.414	16.226	17.716	1.00 20.12	Α

	ATOM	İ075	CG1	ILE A	201		52.880	14.395	18.636	1.00 20.03	A
	ATOM	1076	CD1	ILE A	201		52.408	13.258	17.745	1.00 22.75	
	ATOM	1077	С	ILE A	201		51.193	17.425	20.270	1.00 19.87	
	ATOM	1078	0	ILE A	201		50.121	17.161	20.817	1.00 20.08	
5	ATOM	1079	N	ILE A	202		51.508	18.633	19.815	1.00 19.94	
	ATOM	1080	CA	ILE A	202		50.601	19.772	19.891	1.00 20.45	
	ATOM	1081	СВ	ILE A	202		51.352	21.040	20.356	1.00 22.21	
	ATOM	1082	CG2	ILE A	202		50.381	22.220	20.470	1.00 22.67	
	ATOM	1083	CG1	ILE A	202		52.033	20.775	21.700	1.00 24.19	
10	ATOM	1084	CD1				52.914	21.920	22.169	1.00 25.39	
	ATOM	1085	С	ILE A	202		50.105	19.999	18.464	1.00 20.71	A
	ATOM	1086	0	ILE A	202		50.910	20.067	17.538	1.00 19.48	A
	ATOM	1087	N	HIS A	203		48.795	20.108	18.270	1.00 18.65	Α
	ATOM	1088	CA	HIS A	203		48.280	20.319	16.919	1.00 18.02	A
15	ATOM	1089	СВ	HIS A	203		46.775	20.057	16.874	1.00 16.31	A
	ATOM	1090	CG	HIS A	203		46.199	20.136	15.495	1.00 18.36	Α
	ATOM	1091	CD2	HIS A	203		46.043	21.186	14.655	1.00 16.42	Α
	ATOM	1092	ND1	HIS A	203		45.759	19.026	14.806	1.00 19.50	A
	ATOM	1093	CE1	HIS A	203		45.359	19.389	13.600	1.00 17.64	A
20	ATOM	1094	NE2	HIS A	203		45.522	20.694	13.483	1.00 20.87	A
	ATOM	1095	С	HIS A	203		48.589	21.738	16.405	1.00 18.92	A
	ATOM	1096	0	HIS A	203		49.073	21.906	15.282	1.00 16.21	A
	ATOM	1097	N	ARG A	204		48.301	22.744	17.232	1.00 18.60	A
	ATOM	1098	CA	ARG A	204		48.552	24.157	16.914	1.00 19.81	A
25	ATOM	1099	CB	ARG A	204		49.998	24.365	16.458	1.00 21.61	A
	ATOM	1100	CG	ARG A	204		51.024	24.137	17.550	1.00 23.82	A
	ATOM	1101	CD	ARG F	204		52.323	24.870	17.252	1.00 27.62	A
	ATOM	1102	NE	ARG A	. 204		52.932	24.449	15.994	1.00 29.43	A
	ATOM .	1103	CZ	ARG A	204		54.125	24.861	15.572	1.00 33.10	A
30	ATOM	1104	NH1	ARG A	204		54.835	25.706	16.311	1.00 32.12	A
	ATOM	1105	NH2	ARG A	204		54.614	24.426	14.418	1.00 30.25	A
	ATOM	1106	С	ARG A	204	•	47.624	24.830	15.905	1.00 20.03	A
	ATOM	1107	0	ARG A	204		47.711	26.038	15.698	1.00 20.88	A
	ATOM	1108	· N	ASP A	205		46.755	24.071	15.255	1.00 18.96	A
35	ATOM	1109	CA	ASP A	205		45.828	24.692	14.325	1.00 17.90	A
	ATOM	1110	CB	ASP A	205		46.418	24.741	12.914	1.00 18.95	A
	ATOM	1111	CG	ASP A	205		45.655	25.688	12.008	1.00 20.36	A
	ATOM	1112	OD1	ASP A	205		44.939	26.560	12.545	1.00 20.35	A
	ATOM	1113	OD2	ASP F			45.772	25.573	10.771	1.00 22.49	A
40	ATOM	1114	С	ASP A			44.500	23.956	14.328	1.00 19.60	A
	ATOM	1115	0	ASP F			43.876	23.751	13.287	1.00 21.53	A
	ATOM	1116	N	LEU F			44.063	23.569	15.521	1.00 18.53	A
	MOTA	1117	CA	LEU A		•	42.813	22.851	15.667	1.00 19.18	A
	MOTA	1118	СВ	LEU F			42.693	22.295	17.087	1.00 18.94	A
45	ATOM	1119	CG	LEU F			41.511	21.358	17.346	1.00 23.10	A
	MOTA	1120		LEU F			41.615	20.142	16.436	1.00 23.01	A
	MOTA	1121	CD2	LEU F			41.504	20.933	18.808	1.00 22.97	A
	MOTA	1122	С	LEU A			41.639	23.772	15.361	1.00 19.05	A
	MOTA	1123,		LEU F		•	41.556	24.880	15.886	1.00 19.25	A
50	ATOM	1124	N	LYS F			40.740	23.307	14.500	1.00 17.54	' A
	MOTA	1125	CA	LYS F			39.564	24.081	14.110	1.00 18.60	A
	ATOM	1126	CB	LYS F			39.980	25.248	13.196	1.00 18.98	A
	MOTA	1127	CG	LYS F			40.786	24.817	11.982	1.00 18.20	A
	ATOM	1128	CD	LYS A			41.246	26.000	11.139	1.00 21.42	A
55	ATOM	1129	CE	LYS P			42.223	25.537	10.062	1.00 23.21	A
	ATOM	1130	NZ	LYS A			42.561	26.604	9.084	1.00 29.61	A
	ATOM	1131	С	LYS A			38.566	23.181	13.388	1.00 18.18	A
	ATOM	1132	0	LYS A			38.921	22.100	12.915	1.00 18.11	A
	MOTA	1133	N	PRO P	208		37.298	23.614	13.293	1.00 20.26	A

	MOTA	1134	CD	PRO F	208		36.713	24.833	13.882	1.00	18.79		Α
•	ATOM	1135	CA	PRO F	208		36.272	22.814	12.616	1.00	19.67		Α
	ATOM	1136	CB	PRO P	208		35.063	23.742	12.608	1.00	19.45		Α
	MOTA	1137	CG	PRO F	208		35.231	24.509	13.891	1.00	21.81		A
5	MOTA	1138	С	PRO F	208		36.674	22.372	11.209	1.00	21.04		A
	MOTA	1139	0	PRO A	208		36.264	21.307	10.751	1.00	21.19		A
	MOTA	1140	N	GLU A	209		37.474	23.188	10.528	1.00	21.69		A
	ATOM	1141	CA	GLU A			37.928	22.872	9.170	1.00	22.64		A
	MOTA	1142	CB	GLU	209		38.644	24.084	8.558	0.50	23.65		AC1
10	MOTA	1143	CG.	GLU	209		39.253	23.825	7.185	0.50	27.24		AC1
	MOTA	1144	CD	GLU	209		40.155	24.958	6.716		29.40		AC1
	MOTA	1145		GLU	209		39.660	26.094	6.553	-	29.68		AC1
	MOTA	1146	OE2		209		41.363	24.711	6.511		30.07		AC1
	MOTA	1147	С	GLU A			38.879	21.668	9.159		22.28		A
15	MOTA	1148	0	GLU A			38.955	20.933	8.170		21.36		A
	ATOM	1149	N	ASN A			39.600	21.490	10.263		19.90		Α
	MOTA	1150	CA	ASN A			40.574	20.412	10.436		19.44		A
	ATOM	1151	CB	ASN A			41.744	20.912	11.287		20.07		A
	ATOM	1152	CG	ASN A			42.746	21.698	10.479		25.77		A
20	MOTA	1153		ASN A			43.571	22.427	11.029		26.73		A
	ATOM	1154		ASN A			42.687	21.548	9.158		25.15		A
	ATOM	1155	С	ASN A			40.005	19.151	11.078		18.63		A
	ATOM	1156	0	ASN A			40.712	18.154	11.234		18.29		A.
25	ATOM	1157	N	ILE A			38.739	19.202	11.469		16.31		A
25	ATOM	1158	CA	ILE A			38.090	18.058	12.085 13.354		15.49 15.40		A A
	ATOM	1159	CB				37.336 36.582	18.488 17.311	13.354		14.59		A
	ATOM	1160 1161		ILE A			38.342	19.046	14.365		15.91		A
	ATOM ATOM	1162		ILE A			37.720	19.669	15.590		15.98		A
30	ATOM	1163	CDI	ILE A			37.120	17.485	11.059		17.26		A
30	ATOM	1164	Ó	ILE A			35.995	17.947	10.926		18.16		A
	ATOM	1165	N	LEU A			37.599	16.486	10.320		15.97		A
	ATOM	1166	CA	LEU A			36.784	15.875	9.274		17.08		A
	ATOM	1167	CB	LEU A			37.685	15.249	8.202		17.78		A
35	ATOM	1168	CG	LEU A			38.785	16.157	7.640		18.92		A
33	ATOM	1169		LEU A			39.476	15.450	6.485		22.09		A
	ATOM	1170		LEU A			38.188	17.482	7.166	1.00	19.91		A
	ATOM	1171	С	LEU A			35.843	14.825	9.837	1.00	18.35		A
	ATOM	1172	0	LEU A	212		35.957	14.433	11.002	1.00	19.39	•	A
40	MOTA	1173	N	LEU A	213		34.915	14.368	9.000	1.00	17.84		Α.
	ATOM	1174	CA	LEU A			33.942	13.362	9.403	.1.00	19.94		Α
	ATOM	1175	CB	LEU A	213		32.556	14.004	9.487	1.00	20.84		A
	ATOM	1176	CG	LEU A	213		32.396	15.059	10.583	1.00	20.31		Α
	ATOM	1177	CD1	LEU A	213		31.124	15.837	10.367		22.75		A
45	ATOM	1178	CD2	LEU A	213		32.379		11.940		23.93		A
	ATOM	1179	С	LEU A	213		33.914	12.187	8.426		20.98		Α
	ATOM	1180	0	LEU A			33.743	12.379	7.218		19.55		A
	MOTA	1181	N	ASN A			34.088	10.970	8.935		20.44		A
	MOTA	1182	CA	ASN A			34.055	9.814	8.049		23.77		A
50	ATOM	1183	CB	ASN A			34.745	8.596	8.674		25.30		A
	MOTA	1184	CG	ASN A		-	34.077	8.127	9.948		32.04		A
	ATOM	1185		ASN A			32.908	8.422	10.206		34.43		A
	MOTA	1186		ASN A			34.818	7.369	10.752		33.85		A
	ATOM	1187	C	ASN A			32.618	9.466	7.693		24.07		A
55	MOTA	1188	0	ASN A			31.672	10.113	8.150		19.94		A
	ATOM	1189	N	GLU A			32.459	8.433	6.879		25.77		A n ·
	ATOM	1190	CA	GLU A			31.138	8.003	6.445		28.69 31.98		A ·
	ATOM	1191	CB	GLU A			31.275	6.796	5.513				A n
	MOTA	1192	CG	GLU A	215		29.970	6.334	4.896	1.00	40.22		A

	MOTA	1193	CD	GLU	A 215		30.182	5.312	3.795	1.00 44.27	А
•	ATOM	1194		LGLU			30.817				
	ATOM	1195		GLU.			29.716				A
	ATOM	1196			A 215		30.188				A
. 5	ATOM	1197				•					A
,					A 215		28.971				A
	MOTA	1198			A 216		30.737			1.00 26.77	A
	ATOM	1199	CA		A 216		29.914	6.953	9.917	1.00 27.28	Α
	ATOM	1200	СB		A 216		30.538	5.795	10.696	1.00 31.27	Α
	ATOM	1201	CG	ASP.	A 216		30.390	4.466	9.979	1.00 37.61	A
10	ATOM	1202	OD1	ASP .	A 216		29.274			1.00 39.45	A
	ATOM	1203		ASP .			31.382			1.00 33.43	A
	ATOM	1204	С		A 216		29.697				
	ATOM	1205	ō		A 216		29.136	7.984		1.00 26.37	A
	ATOM	1206			A 217				11.950	1.00 25.73	A
15			N				30.156	9.306	10.441	1.00 23.02	Α
13	ATOM	1207	CA		A 217		30.015		11.218	1.00 21.83	Α
	ATOM	1208	CB		A 217		28.537	10.789	11.517	1.00 23.24	A
	MOTA	1209	CG		A 217		27.742	11.186	10.274	1.00 22.98	A
	ATOM	1210	SD	MET I	A 217		28.464	12.616	9.430	1.00 27.57	A
	ATOM	1211	CE	MET A	A 217		27.679	13.974	10.332	1.00 26.68	A
20	ATOM	1212	С		A 217		30.844	10.618	12.502	1.00 21.51	· A
	ATOM	1213	0		A 217		30.474	11.323	13.440		
	ATOM	1214	N		A 218		31.957			1.00 18.62	A
	ATOM	1215			A 218			9.892	12.544	1.00 20.10	Α
	ATOM		CA				32.873	9.964	13.678	1.00 19.86	. A
25		1216	CB	HIS A			33.482	8.594	13.977	1.00 20.21	Α
25	ATOM	1217	CG		1 218		32.551	7.667	14.698	1.00 22.40	A
	ATOM	1218		HIS A			31.910	6.547	14.287	1.00 21.27	Α
	ATOM	1219		HIS A			32.177	7.863	16.011	1.00 19.59	A
	ATOM	1220	CE1	HIS A	1 218		31.348	6.902	16.379	1.00 21.88	A
	ATOM	1221	NE2	HIS A	218		31.168	6.091	15.351	1.00 22.08	A
30	MOTA	1222	С	HIS A			33.947	10.921	13.172	1.00 19.10	A
	ATOM	1223	0	HIS A			34:170	11.004	11.965	1.00 20.31	
	ATOM	1224	N	ILE A			34.617	11.638			A
	ATOM	1225	CA	ILE A					14.067	1.00 17.21	. A
	ATOM	1226		ILE F			35.628	12.586	13.618	1.00 15.26	Α
35			CB				35.987	13.614	14.716	1.00 15.38	A
33	ATOM	1227		ILE P			34.722	14.305	15.221		A
•	ATOM	1228		ILE A			36.734	12.919	15.864	1.00 14.46	Α
	ATOM	1229		ILE A			37.279	13.885	16.911	1.00 13.74	A
	ATOM	1230	С	ILE A	219		36.929	11.944	13.161	1.00 16.21	A
	ATOM	1231	0	ILE A	219		37.238	10.799	13.500	1.00 15.88	A
40	MOTA	1232	N	GLN A	220		37.677	12.711	12.378	1.00 15.62	A
	ATOM	1233	CA	GLN A	220		38.980	12.316	11.876	1.00 17.84	A
	ATOM	1234	CB	GLN A	220		38.872	11.595	10.525	1.00 20.00	A
	ATOM	1235	CG	GLN A			38.463	10.129	10.659	1.00 26.97	
•	ATOM	1236	CD	GLN A			38.648				A
45	ATOM	400=		GLN A			37.968		9.372	1.00 29.95	A
-13	ATOM									1.00 33.12	A
		1238		GLN A			39.578	8.393	9.389	1.00 30.47	A
	ATOM	1239	С	GLN A			39.757	13.610	11.735	1.00 17.00	A
	ATOM	1240	0	GLN A			39.609	14.339	10.751	1.00 18.27	A
	ATOM	1241	N	ILE A			40.566	13.906	12.746	1.00 14.34	A
<i>5</i> 0	ATOM	1242	CA	ILE A	221		41.361	15.120	12.753	1.00 14.46	A
	ATOM	1243	CB	ILE A	221		41.867	15.416	14.175	1.00 12.30	A
	ATOM	1244	CG2	ILE A	221		42.764	16.656	14.167	1.00 14.78	A
	ATOM	1245		ILE A			40.660	15.613	15.102	1.00 14.78	
	ATOM	1246		ILE A			41.003	15.901	16.543		A
55	ATOM	1247	C	ILE A						1.00 15.06	A
J.J							42.536	14.996	11.783	1.00 15.44	A
	MOTA	1248	0	ILE A			43.106	13.915	11.613	1.00 13.93	A
	ATOM	1249		THR A			42.877	16.101	11.127	1.00 15.36	A
	ATOM	1250		THR A			43.980	16.098	10.174	1.00 17.52	A
	ATOM	1251	CB	THR A	222		43.470	15.836	8.750	1.00 19.92	A

	ATOM	1252	OG1	THR A	222		44.587	15.637	7.875	1.00 18.	78 A
	ATOM	1253	CĠ2	THR A	222		42.630	17.018	8.257	1.00 18.3	
	ATOM	1254	С	THR A			44.735	17.428	10.192	1.00 19.0	
	ATOM	1255	0	THR A			44.509	18.257	11.084	1.00 18.5	
5	ATOM	1256	N	ASP A			45.630	17.610	9.216	1.00 18.6	
	ATOM	1257	CA	ASP A			46.440	18.825	9.069	1.00 20.3	
	ATOM	1258	СВ	ASP A			45.532	20.065	9.108	1.00 23.5	
	ATOM	1259	CG	ASP A			46.248	21.335	8.670	1.00 27.0	
	ATOM	1260		ASP A			47.283	21.227	7.975	1.00 26.2	
10	ATOM	1261		ASP A			45.765	22.438	9.009	1.00 26.1	
	ATOM	1262	C	ASP A			47.516	18.913	10.150	1.00 21.7	
	ATOM	1263	Ö	ASP A			47.439	19.751	11.055	1.00 21.7	
	ATOM	1264	N	PHE A			48.535	18.063	10.027	1.00 20.7	
	ATOM	1265	CA	PHE A			49.611	17.988	11.009	1.00 20.1	
15	ATOM	1266	CB	PHE A			49.805	16.527	11.424	1.00 20.6	
10	ATOM	1267	CG	PHE A			48.682	15.991	12.263	1.00 20.0	
	ATOM	1268		PHE A			48.598	16.312	13.614	1.00 21.9	
	ATOM	1269		PHE A			47.681	15.212	11.693	1.00 23.0	
	ATOM	1270		PHE A			47.528	15.868	14.389	1.00 22.2	
20	ATOM	1271		PHE A		•	46.606	14.763	12.457	1.00 23.3	
20	ATOM	1272	CZ	PHE A			46.530	15.093	13.807	1.00 21.3	
	ATOM	1273	C	PHE A			50.957	18.583	10.619	1.00 22.0	
	MOTA	1274	0	PHE A			51.905	18.547	11.407	1.00 20.7	
	ATOM	1275	.И	GLY A		•	51.049	19.125	9.412	1.00 20.7	
25	ATOM	1276	CA	GLY A			52.301	19.713	8.981	1.00 22.6	
23	ATOM	1277	C	GLY A			52.742	20.822	9.920	1.00 24.9	
	ATOM	1278	o	GLY A			53.939	21.041	10.122	1.00 24.5	
	ATOM	1279	N	THR A			51.779	21.524	10.508	1.00 23.5	
	ATOM	1280	CA	THR A			52.106	22.613	11.416	1.00 25.1	
30	ATOM	1281	СВ	THR A			51.199	23.829	11.160	1.00 24.7	
-	ATOM	1282	OG1	THR A			49.831	23.410	11.113	1.00, 22.6	
	ATOM	1283		THR A			51.571	24.490	9.834	1.00 25.0	
	ATOM	1284	С	THR A			52.046	22.233	12.894	1.00 25.7	
	ATOM	1285	ō	THR A		•	52.019		,13.768	1.00 24.5	
35	ATOM	1286	N	ALA A			52.037	20.935	13.173	1.00 24.9	7 A
	MOTA	1287	CA	ALA A			52.004	20.475	14.550	1.00 25.4	9 A
	ATOM	1288	СВ	ALA A			51.659	18.993	14.607	1.00 22.8	15 A .
	ATOM	1289	С	ALA A			53.384	20.715	15.149	1.00 27.7	'0 A
	ATOM	1290	0	ALA A	227		54.331	21.047	14.435	1.00 26.6	0 A
40	ATOM	1291	N	LYS A	228		53.491	20.558	16.461	1.00 28.5	3 A
	ATOM	1292	CA	LYS A	228		54.760	20.745	17.149	1.00 32.1	.2 A
	ATOM	1293	CB	LYS A	228		54.699	21.974	18.054	1.00 33.8	1 A
	ATOM	1294	CG	LYS A	228		56.007	22.294	18.765	1.00 41.2	3 A
	ATOM	1295	CD	LYS A	228		57.082	22.725	17.768	1.00 47.5	
45	ATOM	1296	CE	LYS A	228		58.401	23.056	18.462	1.00 49.8	2 A
	ATOM	1297	NZ	LYS A	228		59.459	23.425	17.480	1.00 51.4	9 A
•	ATOM	1298	С	LYS A	228		55.019	19.504	17.985	1.00 33.2	.5 A
	ATOM	1299	0	LYS A	228		54.190	19.129	18.815	1.00 33.7	
	MOTA	1300	N	VAL A	229		56.159	18.860	17.756	1.00 33.6	
50	ATOM	1301	CA	VAL A			56.516	17.661	18.501	1.00 34.6	
	MOTA	1302	CB	VAL A			57.248	16.646	17.609	1.00 33.5	
	ATOM	1303		VAL A			57.619	15.419	18.415	1.00 32.3	
	ATOM	1304	CG2	VAL A			56.370	16.264	16.436	1.00 34.2	
	MOTA	1305	С	VAL A			57.420	18.035	19.668	1.00 37.5	
55	ATOM	1306	0	VAL A			58.581	18.392	19.474	1.00 35.9	
	MOTA	1307	N	LEU A			56.877	17.948	20.878	1.00 40.5	
	MOTA	1308	CA	LEU A			57.615	18.289	22.088	1.00 46.1	
	ATOM	1309	CB	LEU A			56.654	18.417	23.270	1.00 44.7	
	ATOM	1310	CG	LEU A	230		55.627	19.545	23.207	1.00 44.5	0 A

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	ATOM	1311	_	LEU .			54.673	19.430	24.383	1.00	44.39	A
	ATOM	1312	CD2	LEU .	1 2	30	56.340	20.885	23.214	1.00	44.81	A
	ATOM	1313	С	LEU :	1 2	30	58.695	17.279	22.440	1.00	50.42	A
	ATOM	1314	0	LEU :	A 2:	30	58.603	16.104	22.089		51.64	A
5	ATOM	1315	N	SER			59.717	17.756	23.145		55.81	A
	ATOM	1316	CA	SER A			60.824	16.914	23.583		61.14	A
	MOTA	1317	CB .	SER I			62.077	17.200	22.750		61.27	A
	ATOM	1318	OG	SER I	1 2:	31	62.444	18.568	22.823	1.00	62.85	A
	ATOM	1319	С	SER I	1 2:	31	61.124	17.126	25.071	1.00	64.65	A
10	ATOM	1320	0	SER Z	1 2	31	61.392	16.164	25.794	1.00	65.70	A
	ATOM	1321	N	PRO 2	1 2:	32	61.081	18.387	25.549	1.00	67.54	A
	ATOM	1322	CD	PRO 2			60.854	19.651	24.823		68.60	A
		1323	CA	PRO Z			61.358	18.655	26.966		68.74	A
	ATOM											
	ATOM	1324	CB	PRO A			61.109	20.158	27.086		68.83	A.
15	MOTA	1325	CG	PRO 2			61.505	20.666	25.737		68.96	Α
	ATOM	1326	С	PRO I			60.460	17.846	27.899	1.00	69.17	A
	ATOM	1327	0	PRO I	1 2:	32	59.335	17.494	27.541	1.00	69.94	Α
	ATOM	1328	N	ALA A	23	37	57.424	23.198	27.637	1.00	80.06	A
	ATOM	1329	CA	ALA A	1 2:	37	56.783	23.047	26.335	1.00	79.29	Α
20	ATOM	1330	СВ	ALA A			55.275	22.907	26.512	1.00	78.64	A
20		1331	C	ALA A			57.092	24.239	25.433		79.07	A
	ATOM			ALA			56.250	25.113	25.249		79.47	A
	ATOM	1332	0									
	MOTA	`1333	N	ALA Z			58.297	24.280	24.871		78.57	A
	MOTA	1334	CA	ALA A	2:	38	58.683	25.383	23.992		78.50	A
25	ATOM	1335	CB	ALA Z	1 2:	38	60.186	25.347	23.728	1.00	78,50	A
	ATOM	1336	Ċ	ALA A	1 2:	38	57.920	25.327	22.673	1.00	78.15	A
	ATOM	1337	0	ALA Z	2	38	57.243	24.341	22.375	1.00	77.96	Α
	ATOM	1338	N	ALA Z			58.027	26.393	21.887	1.00	77.28	А
	ATOM	1339	CA	ALA Z			57.338	26.452	20.603		76.27	A
30	ATOM	1340	CB.	ALA A			55.849	26.489	20.827		76.61	A
50			CD.	ALA			57.766	27.667	19.793		75.38	A
	ATOM	1341									75.89	A
	ATOM	1342	0	ALA I			58.955	27.955	19.700			
	MOTA	1343	N	ASN A			56.781	28.357	19.214		73.95	A
	ATOM	1344	CA	ASN 2			56.967	29.553	18.389		71.07	A
35	ATOM	1345	CB	ASN A	A 2	40	58.151	30.400	18.874	1.00	71.47	A
	MOTA	1346	CG	ASN Z	4 2	40	59.459	30.055	18.174	1.00	72.06	A
	ATOM	1347	OD1	ASN Z	1 2	40	59.575	30.149	16.943	1.00	72.03	Α
	ATOM	1348		ASN Z			60.470	29.665	18.964	1.00	71.91	A
	ATOM	1349	C	ASN A			57.188	29.178	16.928	1.00	69.41	A
40	ATOM	1350	Ö	ASN A			57.480	28.024	16.624		70.09	A
40				ALA A			57.055	30.165	16.038		66.62	A
`	ATOM	1351	N				57.246		14.585		63.94	A
	ATOM	1352	CA	ALA A				30.013				A
	MOTA	1353	С	ALA A			55.952	30.080	13.772		60.63	
	MOTA	1354	0	ALA Z	1 2	41	55.840	30.880	12.845		61.29	A
45	ATOM	1355	CB	ALA A	1 24	41	57.979	28.704	14.246		65.23	A
	MOTA	1356	N	PHE A	.24	42	54.984	29.236	14.113	1.00	56.72	A
	ATOM	1357	CA	PHE A	24	42	53.712	29.196	13.394	1.00	52.53	A
	ATOM	1358	СВ	PHE 2			53.419	27.767	12.923	1.00	49.14	Α
	ATOM	1359	CG	PHE A			52.040	27.590	12.354		47.38	A
50		1360		PHE A			51.731	28.067	11.085		47.69	A
50	MOTA							26.975	13.102		45.45	A
	MOTA	1361		PHE A			51.038					
	MOTA	1362		PHE A			50.445	27.937	10.565		46.75	Α
	MOTA	1363		PHE 2			49.751	26.840	12.594		45.41	A
	MOTA	1364	CZ	PHE -			49.453	27.323	11.322		46.55	A
55	MOTA	1365	С	PHE A	24	42	52.534	29.688	14.229		50.08	A
	ATOM	1366	0	PHE A			52.502	29.505	15.444	1.00	49.86	Α
	ATOM	1367	N	VAL A			51.566	30.305	13.557	1.00	47.67	Α
	ATOM	1368	CA	VAL 2			50.355	30.809	14.200		46.21	A
			CB	VAL Z			50.340	32.352	14.258		47.36	A
	MOTA	1369	CD	AWP 1	. 4	2.0	30.340	JE.JJE	23.200	1.00	.,.50	**

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	ATOM	1370	CG1	VAL	Α	243		49.012	32.844	14.825	1.00 47.54	A
	ATOM	1371		VAL				51.497	32.842	15.109	1.00 48.50	A
	ATOM	1372	C	VAL				49.150	30.342	13.389	1.00 44.12	A
	ATOM	1373	o	VAL				48.956	30.765	12.247	1.00 44.46	A
5	ATOM	1374	N	GLY				48.348	29.467	13.985	1.00 40.48	A
3		1375	CA	GLY				47.176	28.941	13.306	1.00 37.65	A
	ATOM		C	GLY				46.101	29,960	12.964	1.00 35.39	A
	ATOM	1376		GLY				46.313	31.168	13.065	1.00 35.92	A
	MOTA	1377	0	THR				44.936	29.463	12.560	1.00 33.30	A
	MOTA	1378	N					43.813	30.312	12.184	1.00 30.20	A
10	MOTA	1379	CA	THR				42.593	29.450	11.829	1.00 32.00	A
	MOTA	1380	CB	THR	A	245				10.755	1.00 32.81	A
	MOTA	1381		THR				42.952	28.573	11.390	1.00 32.31	A
•	MOTA	1382	CG2	THR				41.419	30.319	13.296	1.00 20.34	A
	MOTA	1383	С	THR	A	245		43.476	31.296		1.00 27.90	A
15	ATOM	1384	0	THR	A	245		43.212	30.907	14.434		A
	ATOM	1385	N	ALA				43.486	32.576	12.938	1.00 25.22	A
	MOTA	1386	CA	ALA	Α	246		43.247	33.675		1.00 23.27	
	ATOM	1387	CB	ALA	Α	246	•	42.956	34.955	13.082	1.00 22.94	A
	ATOM	1388	C	ALA				42.178	33.475	-14.934	1.00 21.27	A
20	ATOM	1389	ō	ALA				42.431	33.705	16.114	1.00 20.93	A
20		1390	N			247		40.988	33.047	14.536	1.00 19.67	A
	ATOM	1391	CA			247		39.911	32.886	15.504	1.00 20.17	A
	MOTA	1392	CB	GLN	••	247		38.608	32.535	14.779	0.50 21.89	AC1
	MOTA		CG	GLN		247		38.522	33.076	13.355	0.50 26.18	AC1
	MOTA	1393				247		37.220	33.794	13.064	0.50 27.30	AC1
25	MOTA	1394	CD	GLN		247		36.172	33.447	13.605	0.50 30.13	AC1
	MOTA	1395	OE1					37.278	34.792	12.189	0.50 28.70	AC1
	ATOM	1396		GLN		247		40.181	31.849	16.595	1.00 19.43	A
	MOTA	1397	С			247			31.883	17.648	1.00 18.93	A
	MOTA	1398	0			247		39.546		16.359	1.00 18.60	A
30	ATOM	1399	N	TYR	Α	248		41.132	30.948		1.00 19.20	A
	ATOM	1400	CA			248		41.441	29.896	17.329	1.00 17.53	A
	ATOM	1401	CB	TYR	A	248		41.333	28.529	16.642	1.00 17.33	A
	ATOM	1402	CG	TYR	A	248		40.013	28.362	15.927		A
	ATOM	1403	CD1	TYR	A	248		38.859	28.010		1.00 17.69	A
35	ATOM	1404	CE1	TYR	A	248		37.617	27.976		1.00 18.18	
23	ATOM	1405	CD2	TYR	A	248		39.897	28.664	14.569	1.00 16.87	A
	ATOM	1406		TYP				38.665	28.635	13.924	1.00 19.17	A
	MOTA	1407	CZ			248		37.527	28.295		1.00 19.46	A
		1408	ОН			248	•	36.299	28.311		1.00 18.98	A
40	ATOM	1409	C			248		42.810	30.039		1.00 20.42	A
40	ATOM		Ö			248		43.208	29.191	18.792	1.00 19.19	A
	ATOM	1410				249		43.523			1.00 20.20	A
	ATOM	1411	N			249		44.841	31.343		1.00 20.91	A
	ATOM	1412	CA			249		45.542			1.00 21.18	A
	ATOM	1413	CB					46.821			1.00 22.45	A
45	MOTA	1414	CG.	I VAI	. P.	249					1.00 24.01	Α
	ATOM	1415	· CG			249		45.862			1.00 21.52	A
	ATOM '	1416	C			249		44.764			1.00 22.72	A
	ATOM	1417	О			249		43.915				A
	ATOM	1418	N			250		45.654			1.00 20.70	A
50	ATOM	1419	CA			250		45.697				A
	MOTA	1420	CB	SE	R F	250		46.370				
	ATOM	1421				A 250		47.692				A
	ATOM	1422				A 250		46.476		2 22.280		A
	MOTA	1423		SE	R I	250)	47.332			1.00 22.77	A
55	ATOM	1424				251		46.180	33.029		_	A
55		1425				A 251		45.163		4 24.433	1.00 22.97	A
	MOTA	1425				A 251		46.893			1.00 22.52	A
	MOTA					A 251		46.233			1.00 23.06	A
	ATOM	1427				A 251		45.726				A
	MOTA	1428	CG	PR	0 2	. Z31	-	43.720	, ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			

	ATOM	1429	С	PRO A	251	4	8.414	34.115	23.907	1.00	22.15	А
	ATOM	1430	0	PRO A			9.143	35.047	23.563		22.62	. A
	ATOM	1431	N	GLU A			8.901	32.966	24.367		20.69	A
	ATOM	1432	CA				0.347	32.772	24.500		21.40	
5	ATOM	1433	СВ	GLU A			0.673	31.382	25.071		20.59	A
,	ATOM	1434	CG	GLU A								A
							9.993	30.232	24.352		21.91	A
	ATOM	1435	CD	GLU A			8.691	29.822	25.014		21.51	A
	ATOM	1436		GLU A			7.989	30.707	25.550		21.46	A
10	ATOM	1437		GLU A			8.367	28.613	24.993		20.23	A
10	MOTA	1438	С	GLU A			1.071	32.970	23.167		22.99	A
	ATOM	1439	0	GLU A			2.191	33.480	23.136		23.17	A
	MOTA	1440	N	LEU A		5	0.441	32.576	22.064		23.00	Α
	MOTA	1441	CA	LEU A	253	5	1.068	32.753	20.758	1.00	25.62	A ·
	ATOM	1442	CB	LEU A	253	5	0.277	32.029	19.669	1.00	26.75	A
15	MOTA	1443	CG	LEU A	253	- 5	0.743	30.620	19.296	1.00	31.87	А
	ATOM	1444	ĊD1	LEU A	253	5	0.433	29.651	20.422	1.00	31.81	A
	MOTA	1445	CD2	LEU A	253	5	0.044	30.179	18.015		31.86	A
	MOTA	1446	Ć	LEU A			1.201	34.228	20.371		26.94	A
	ATOM	1447	0	LEU A			2.107	34.601	19.626		27.09	A
20	ATOM	1448	N	LEU A			0.297	35.059	20.877		25.83	A
	ATOM	1449	CA	LEU A			0.297	36.485	20.564		27.26	· A
	ATOM	1450	СВ	LEU A			8.858	37.006	20.564		25.84	A
	ATOM	1451	CG	LEU A			7.882	36.290	19.621		24.69	· A
	ATOM	1452		LEU A			6.459	36.724				
25	ATOM	1453							19.932		23.64	. A
23				LEU A			8.236	36.597	18.177		24.24	A
	ATOM	1454	C	LEU A			1.134	37.314	21.537		30.62	A
	ATOM	1455	0	LEU A			1.633	38.383	21.187		32.35	A
	ATOM	1456	N	THR A			1.292	36.821	22.758		32.47	A
~~	ATOM	1457	CA	THR A			2.056	37.547	23.759		36.70	A
30	ATOM	1458	CB	THR A			1.368	37.478	25.127		34.51	A
	ATOM	1459	OG1			5.	1.188	36.106	25.494	1.00	35.49	A
	MOTA	1460	CG2	THR A	255		0.013	38.166	25.077	1.00	33.40	Α
. •	MOTA	1461	С	THR A			3.477	37.035	23.910		40.09	A
	MOTA	1462	0	THR A	255	5	4.430	37.793	23.772	1.00	43.69	A
35	MOTA	1463	N	GLU A	256	5	3.617	35.747	24.189	1.00	44.77	A
	ATOM	1464	CA	GLU A	256	5	4.932	35.144	24.382	1.00	49.15	A
	ATOM	1465	CB	GLU A	256	5	4.866	34.143	25.534	1.00	51.24	Α
	MOTA	1466	CG	GLU A	256	· 5·	4.514	34.786	26.862	1.00	56.03	Α
	ATOM	1467	CD	GLU A	256	5	4.053	33.780	27.893	1.00	58.83	A
40	MOTA	1468	OE1	GLU A	256	5	4.766	32.776	28.107	1.00	62.13	A
	ATOM	1469	OE2	GLU A	256	5.	2.979	33.996	28.494		60.34	A
	ATOM	1470	С	GLU A	256		5.475	34.456	23.137		50.09	A
	ATOM	1471	0	GLU A	-		6.616	33.995	23.127		50.42	A
	ATOM	1472	N	LYS A			4.658	34.389	22.090		51.21	A
45	ATOM	1473	CA	LYS A			5.064	33.746	20.845		51.22	A
	ATOM	1474	CB	LYS A			5.244	34.502	20.227		53.28	A
	ATOM	1475	CG	LYS A			5.558	34.125	18.790		55.19	A
	ATOM	1476	CD	LYS A			7.709	34.961	18.253		57.52	
	ATOM	1477	CE									A
50	ATOM	1478		LYS A			7.952	34.694	16.777		58.52	A
50	ATOM		NZ	LYS A			3.290	33.268	16.515		60.88	A
		1479	С	LYS A			5.467	32.302	21.138		50.74	A
	ATOM	1480	0	LYS A			5.432	31.790	20.577		52.26	A
	ATOM	1481	N	SER A			1.721	31.654	22.027		48.07	A
~~	ATOM	1482	CA	SER A			1.999	30.273	22.402		46.87	A
55	ATOM	1483	CB	SER A			5.590	30.229	23.812		48.88	A
	ATOM	1484	OG	SER A			1.741	30.892	24.734		53.14	Α
	MOTA	1485	С	SER A			3.735	29.415	22.342			A
	ATOM	1486	0	SER A			2.617	29.932	22.417	1.00	44.17	A
	ATOM	1487	N	ALA A	259	53	3.917	28.105	22.204	1.00	38.30	A

	ATOM	1488	CA	ALA	Α	259		52.793	27.180	22.127	1.00 34.73	A
	ATOM	1489	CB	ALA	Α	259	•	52.551	26.779	20.684	1.00 34.16	· A
	ATOM	1490	С	ALA				53.042	25.940	22.977	1.00 32.34	A
	ATOM	1491	0	ALA				54.172	25.459	23.086	1.00 31.81	A
5	ATOM	1492	N	CYS				51.975	25.428	23.579	1.00 28.58	A
-	ATOM	1493	CA	CYS				52.056	24.244	24.425	1.00 26.27	Α -
	ATOM	1494	CB	CYS				52.183	24.654	25.892	1.00 26.53	A
	ATOM	1495	SG	CYS				50.846	25.739	26.469	1.00 32.91	A
	ATOM	1496	C	CYS				50.786	23.435	24.224	1.00 22.83	A
10	ATOM	1497	o	CYS				49.892	23.856	23.495	1.00 22.14	A
10	ATOM	1498	N	LYS				50.706	22.277	24.868	1.00 20.02	A
	ATOM	1499	CA	LYS				49.526	21.434	24.744	1.00 20.65	A
	ATOM	1500	CB	LYS				49.619	20.243	25.696	1.00 23.28	A
	ATOM	1501	CG	LYS				50.716		25.347	1.00 27.44	A
15		1501	CD	LYS				50.710	18.117	26.350	1.00 29.98	A
15	ATOM	1502	CE	LYS			,	51.922	17.203	26.134	1.00 32.34	A
	ATOM	1503	NZ	LYS				51.940	16.121	27.153	1.00 33.28	A
	ATOM			LYS				48.268	22.229	25.062	1.00 19.20	A
	ATOM	1505	C	LYS				47.253	22.092	24.387	1.00 18.08	A
20	ATOM	1506	0	SER				48.358	23.068	26.089	1.00 16.92	A
20	ATOM	1507	N	SER				47.235	23.883	26.534	1.00 18.13	A
	ATOM	1508	CA	SER				47.233	24.698	27,770	1.00 18.27	A
	ATOM	1509	CB	SER				46.517	25.258	28.421	1.00 22.53	A
	ATOM	1510	OG C	SER				46.736	24.811	25.424	1.00 16.77	A
25	ATOM	1511 1512		SER				45.591	25.254	25.450	1.00 15.69	A
25	MOTA	1512	N O	SER				47.595	25.118	24.456	1.00 16.44	A
	ATOM	1514	CA	SER				47.175	25.970	23.347	1.00 16.89	A
	ATOM ATOM	1514	CB			263		48.340	26.228	22.382	1.00 18.49	A
	ATOM	1516	OG	SER				49.402	26.909	23.031	1.00 22.10	A
30	ATOM	1517	C			263		46.040	25.257	22.612	1.00 17.79	. A
30	ATOM	1518	Ö			263		45.099	25.898	22.148	1.00 17.57	A
	MOTA	1519	N	ASP				46.119	23.928	22.517	1.00 16.30	A
	ATOM	1520	CA	ASP				45.069	23.166	21.836	1.00 16.72	A
	ATOM	1521	СВ			264		45.483	21.704	21.620	1.00 15.92	A
35	ATOM	1522	CG	ASP				46.544	21.539	20.548	1.00 17.93	A
55	ATOM	1523		ASP				46.642	22.412	19.661	1.00 16.78	A
	ATOM	1524		ASP				47.265	20.515	20.579	1.00 16.64	A
	ATOM	1525	C	ASP				43.773	23.194	22.646	1.00 17.67	A
	ATOM	1526	0			264		42.681	23.197	22.076	1.00 18.27	A
40	ATOM	1527	N	LEU	Α	265		43.898	23.205	23.974	1.00 15.49	A
	ATOM	1528	CA	LEU	Α	265		42.730	23.232	24.849	1.00 14.75	A
	ATOM	1529	CB			265		43.147	23.038	26.313	1.00 11.38	A
	MOTA	1530	CG	LEU	Α	265		43.711	21.641	26.621	1.00 14.04	Α
	ATOM	1531	CD1	LEU	Α	265		44.249	21.579	28.052	1.00 13.96	A
45	MOTA	1532	CD2	LEU	Α	265		42.619	20.603	26.416	1.00 11.62	Α
	ATOM	1533	С	LEU	Α	265		41.999	24.557	24.675	1.00 15.13	Α
	MOTA	1534	0	LEU	Α	265		40.777	24.620	24.785	1.00 16.75	A
	MOTA	1535	N	TRP	Α	266		42.746	25.622	24.405	1.00 16.08	A
	ATOM	1536	CA	TRP	Α	266		42.118	26.918	24.184	1.00 16.96	A
50	ATOM	1537	CB	TRP	Α	266		43.176	28.015	24.023	1.00 17.28	A
	MOTA	1538	CG			266		42.618	29.326	23.521	1.00 20.54	A
	MOTA	1539		TRP				42.313	30.490	24.301	1.00 20.07	A
	ATOM	1540		TRP				41.782	31.459	23.417	1.00 20.46	A
	ATOM	1541		TRP				42.435	30.810	25.660	1.00 20.68	A
55	ATOM	1542		TRP				42.270	29.631	22.231	1.00 19.53	A
	ATOM	1543		TRP				41.769	30.908	22.163	1.00 19.61	A
•	ATOM	1544		TRP				41.372	32.727	23.850	1.00 20.90	A
	MOTA	1545		TRP				42.026	32.073	26.091	1.00 19.45	A
	ATOM	1546	CH2	TRP	A	266		41.501	33.015	25.185	1.00 20.71	A

	MOTA	1547	С	TRP	A	266	41.284	26.795	22.913	1.00 17	.22	A
	ATOM '	1548	0	TRP	Α	266	40.139	27.240	22.863	1.00 18	.03	Α
	ATOM	1549	N	ALA	A	267	41.863	26.181	21.886	1.00 17		Α
	ATOM	1550	CA	ALA	Α	267	41.155	25.990	20.626	1.00 16	.16	Α
5	ATOM	1551	CB	ALA	Α	267	42.050	25.290	19.621	1.00 14	.28	Α
	ATOM	1552	С	ALA	Α	267	39.901	25.159	20.891	1.00 16		Α
	ATOM	1553	0	ALA	A	267	38.835	25.436	20.346	1.00 16		Ά
	ATOM	1554	N	LEU	Α	268	40.031	24.144	21.739	1.00 16		A
	ATOM	1555	CA	LEU			38.890	23.299	22.084	1.00 17		A
10	ATOM	1556	СВ	LEU			39.292	22.260	23.139	1.00 15		A
	ATOM	1557	CG			268 .	38.158	21.429	23.754	1.00 19		A
	ATOM	1558		LEU			37.505	20.578	22.678	1.00 16		A
	ATOM	1559		LEU			38.718	20.537	24.881	1.00 17		A
	ATOM	1560	С	LEU			37.766	24.179	22.628	1.00 15		Α
15	ATOM	1561	ō	LEU			36.603	24.031	22.247	1.00 15		A
	ATOM	1562	N	GLY			38.119	25.099	23.520	1.00 14		Α
	ATOM	1563	CA	GLY			37.124	25.989	24.092	1.00 13		Α
	ATOM	1564	C	GLY			36.406	26.808	23.031	1.00 14		A
	ATOM	1565	Ö	GLY			35.193	27.014	23.114	1.00 14		A
20	ATOM	1566	N	CYS			37.146	27.279	22.030	1.00 13		Α
20	ATOM	1567	CA	CYS			36.539	28.061	20.958	1.00 16		A
	ATOM	1568	СВ	CYS			37.611	28.634	20.023	1.00 15		A
	ATOM	1569	SG	CYS			38.751	29.810	20.780	1.00 20		A
	ATOM	1570	C	CYS			35.598	27.175	20.140	1.00 17		Α
25	ATOM	1571	0	CYS			34.516	27.604	19.741	1.00 18		A
23	ATOM	1572	N	ILE			36.022	25.939	19.887	1.00 16		A
	ATOM	1573	CA	ILE			35.221	25.004	19.104	1.00 16		Α
	ATOM		CB	ILE			36.038	23.741	18.778	1.00 16		Α
	ATOM	1575		ILE			35.155	22.694	18.102	1.00 16	.34	Α
30	ATOM	1576		ILE			37.222	24.129	17.882	1.00 15	.59	Α
	ATOM	1577		ILE			38.239	23.018	17.690	1.00 14	.88	Α
	ATOM	1578	С	ILE			33.920	24.626	19.809	1.00 16	.74	Α
	MOTA	1579	0	ILE	Α	271	32.865	24.576	19.179	1.00 17	.12	Α
	ATOM	1580	N	ILE	Α	272	33.990	24.357	21.111	1.00 16	.13	Α
35	ATOM	1581	CA	ILE	Α	272	32.785	24.021	21.862	1.00 18	.30	Α
	ATOM	1582	СВ	ILE	Α	272	33.097	23.747	23.346	1.00 17	.77	Α
	ATOM	1583	CG2	ILE '	Ά	272	31.796	23.666	24.152	1.00 17	.96	Α
	ATOM	1584	CG1	ILE	Α	272	33.877	22.437	23.481	1.00 19	.55	Α
	ATOM	1585	CD1	ILE	A	272	34.446	22.217	24.886	1.00 18	. 64	Α
40	ATOM	1586	С	ILE	Α	272	31.824	25.207	21.776	1.00 19	.51	Α
	ATOM	1587	0	ILE	Α	272	30.624	25.037	21.554	1.00 20	. 44	A
	ATOM	1588	N	TYR	Α	273	32.362	26.409	21.947	1.00 18		Α
	ATOM	1589	CA	TYR	Α	273	31.553	27.615	21.881	1.00 20	.48	Α
	ATOM	1590	CB	TYŔ	A	273	32.418	28.847	22.162	1.00 18		Α
45	ATOM	1591	CG	TYR	A	273	31.663	30.161	22.125	1.00 20		A
	ATOM	1592	CD1	TYR	Α	273	31.229	30.709	20.916	1.00 20		Α
	ATOM	1593	CE1	TYR	Α	273	30.536	31.917	20.880	1.00 20		Α
	ATOM	1594	CD2	TYR	A	273	31.383	30.857	23.302	1.00 19		A
	ATOM	1595	CE2	TYR	Α	273	30.691	32.062	23.280	1.00 20		Α
50	MOTA	1596	CZ	TYR	A	273	30.271	32.587	22.067	1.00 21		A
	ATOM	1597	OH	TYR	A	273	29.588	33.776	22.049	1.00 21		Α
	MOTA	1598	С	TYR	Α	273	30.902	27.730	20.507	1.00 21		Α
	MOTA	1599	0	TYR	Α	273	29.719	28.049	20.401	1.00 22		A
	MOTA	1600	N	GLN	A	274	31.676	27.454	19.461	1.00 21		A
55	ATOM	1601	CA	GLN			31.176	27.538	18.095	1.00 21		A
	ATOM	1602	CB	GLN			32.323	27.341	17.097	1.00 21		A
	ATOM	1603	CG	GLN			31.934	27.596	15.645	1.00 23		A
	ATOM	1604	CD	GLN			33.131	27.588	14.706	1.00 24		A
	ATOM	1605	OE1	GLN	A	274	34.276	27.446	15.139	1.00 22	. 51	Α

	ATOM	1606	NE2	GLN	A	274		32.870	27.750	13.413	1.00 22	2.96		A
	ATOM	1607	С	GLN	A	274		30.076	26.517	17.828	1.00 2	1.51		A
	MOTA	1608	0	GLN	Α	274		29.123	26.806	17.108	1.00 20).50		Α
	ATOM	1609	N	LEU	Α	275		30.207	25.324	18.403	1.00 21	.44		Α
5	ATOM	1610	CA	LEU	Α	275		29.196	24.282	18.208	1.00 20).95		Α
	ATOM	1611	CB	LEU	Α	275		29.645	22.958	18.846	1.00 19).11		Α
	ATOM	1612	CG	LEU	Α	275		30.775	22.182	18.159	1.00 2	.43		Α
	ATOM	1613	CD1	LEU	Α	275		31.118	20.936	18.963	1.00 17	7.64		Α
	MOTA	1614	CD2	LEU				30.342	21.795	16.754	1.00 20	34		A
10	MOTA	1615	С	LEU				27.860	24.697	18.815	1.00 21		•	Α
	MOTA	1616	0	LEU	Α	275		26.802	24.461	18.229	1.00 19	3.75		Α
	MOTA	1617	N	VAL	A	276		27.921	25.322	19.987	1.00 19			Ą
	MOTA	1618	CA	VAL				26.724	25.750	20.702	1.00 22			Α
	MOTA	1619	CB	VAL	A	276		27.011	25.882	22.217	1.00 20			A
15	MOTA	1620		VAL				25.742	26.291	22.957	1.00 19			A
	MOTA	1621	CG2	VAL				27,550	24.558	22.766	1.00 19			Α
	MOTA	1622	С	VAL				26.127	27.075	20.211	1.00 23			A
	MOTA	1623	0	VAL	A	276		24.910	27.199	20.070	1.00 24			Α
	MOTA	1624	N	ALA				26.983	28.062	19.965	1.00 24			A
20	ATOM	1625	CA	ALA				26.533	29.374	19.518	1.00 24			A
	MOTA	1626	CB	ALA				27.504	30.444	19.999	1.00 24		•	A
	MOTA	1627	С	ALA				26.378	29.458	18.005	1.00 25			A
	MOTA	1628	0	ALA				25.577	30.242	17.502	1.00 26			A
	MOTA	1629	И	GLY				27.142	28.651	17.280	1.00 25			A
25	ATOM	1630	CA	GLY				27.062	28.673	15.834	1.00 25			A
	ATOM	1631	С	GLY				28.163	29.524	15.231	1.00 26			A
	MOTA	1632	0	GLY			•	28.374	29.510	14.015	1.00 28		•	A
	MOTA	1633	N	LEU				28.866	30.262	1,6.086	1.00 24			A
	ATOM	1634	CA	LEU				29.962	31.130	15.656	1.00 25			A
30	MOTA	1635	CB	LEU				29.468	32.575	15.500	1.00 25			A A
	ATOM	1636	CG	LEU				28.364	32.899	14.490	1.00 28			A
	ATOM	1637		LEU				27.922	34.344	14.684	1.00 26			A
	ATOM	1638		LEU				28.862	32.670	13.071 16.687	1.00 23			A
25	ATOM	1639	С	LEU				31.093 30.848	31.116 30.994	17.882	1.00 24			A
35	ATOM	1640	0	LEU				32.349	31.239	16.236	1.00 23			A
	ATOM	1641	И	PRO PRO				32.831	31.404	14.855	1.00 22			A
	ATOM	1642	CD CA	PRO				33.464	31.239	17.189	1.00 23			A
	ATOM	1643 1644	CB	PRO				34.692	31.293	16.282	1.00 23			A
40	ATOM ATOM	1645	CG	PRO				34.189	32.020	15.073	1.00 24			A
40	ATOM	1646	C	PRO				33.353	32.444	18.137	1.00 22			A.
	ATOM	1647	o	PRO				32.750	33.457	17.788	1.00 22			A
	ATOM	1648	N	PRO				33.939	32.344	19.345	1.00 23			Α
	ATOM	1649	CD	PRO				34.810	31.223	19.734	1.00 21			A
45	ATOM	1650	CA	PRO				33.935	33.375	20.395	1.00 23	3.67		A.
.5	ATOM	1651	CB	PRO				34.781	32.751	21.509	1.00 24		•	Α
	ATOM	1652	CG	PRO				34.749	31.287	21.219	1.00 25			Ä
	ATOM	1653	C	PRO				34.481	34.752	20.017	1.00 23			Α
	ATOM	1654	ō	PRO				33.869	35.781	20.317	1.00 23			Α
50	ATOM	1655	N	PHE				35.644	34.763	19.379	1.00 22	2.17		A
•	ATOM	1656	CA	PHE				36.293	36.007	18.998	1.00 23			A
	ATOM	1657	CB	PHE				37.765	35.943	19.406	1.00 21	1.01		Α
	ATOM	1658	CG	PHE				37.975	35.482	20.822	1.00 22			Α
	ATOM	1659		PHE				37.806	36.361	21.888	1.00 20	0.06		Α
55	ATOM	1660		PHE				38.291	34.151	21.093	1.00 20			Α
	ATOM	1661		PHE				37.947	35.921	23.206	1.00 22			Α
	MOTA	1662	CE2	PHE	A	282		38.433	33.702	22.405	1.00 20			Α
	ATOM	1663	CZ	PHE	A	282		38.261	34.590	23.466	1.00 19			A
	ATOM	1664	С	PHE	A	282		36.169	36.263	17.503	1.00 24	1.39		A

	ATOM	1665	0	PHE	A 282	2 36.802 ⁻	35.585	16.694	1.00 25.80	А
	ATOM	1666	N		A 283		37.248	17.142	1.00 23.80	A
	ATOM	1667	CA		A 283		37.594	15.741	1.00 24.33	
	ATOM	1668	СВ		A 283		37.209	15.316		A
5	ATOM	1669	CG		A 283		35.808	15.724	1.00 28.91	A
,	ATOM	1670			A 283				1.00 30.27	A
			CD				35.493	15.188	1.00 33.36	A
	ATOM	1671	NE		A 283		36.392	15.733	1.00 32.76	Α
	ATOM	1672	CZ		A 283		36.287	16.952	1.00 34.79	A
10	ATOM			ARG			35.317	17.768	1.00 35.77	A
10	ATOM	1674		2 ARG			37.156	17.359	1.00 36.12	A
	ATOM	1675	С		A 283		39.096	15.544	1.00 26.47	A
	ATOM	1676	0		A 283		39.888	16.438	1.00 26.28	A
• •	ATOM	1677	N		A 284		39.486	14.373	1.00 26.70	· A
	ATOM	1678	CA		A 284		40.899	14.079	1.00 27.84	A
15	ATOM	1679	CB	ALA .	A 284	37.188	41.442	14.914	1.00 26.24	A
	ATOM	1680	С	ALA .	A 284	36.327	41.077	12.602	1.00 28.35	A
	MOTA	1681	0	ALA .	A 284	36.560	40.101	11.891	1.00 29.91	А
	MOTA	1682	N	GLY .	A 285	36.332	42.329	12.153	1.00 29.29	A
	MOTA	1683	CA	GLY .	A 285	36.577	42.631	10.753	1.00 29.52	A
20	ATOM	1684	С	GLY .	A 285	37.893	42.156	10.168	1.00 30.12	A
•	MOTA	1685	0	GLY .	A 285	37.974	41.862	8.976	1.00 30.60	A
	MOTA	1686	N	ASN .	A 286		42.097	10.983	1.00 28.49	A
	ATOM	1687	CA		A 286		41.644	10.489	1.00 26.71	A
	ATOM	1688	CB		A 286		42.825	9.945	1.00 26.11	A
25	ATOM	1689	CG		A 286		43.900	10.990	1.00 27.83	A
	ATOM	1690		ASN			43.631	12.049	1.00 27.84	A
	ATOM	1691		ASN			45.131	10.685	1.00 27.04	A
	ATOM	1692	C		A 286		40.924	11.584	1.00 25.33	A
	ATOM	1693	ŏ		A 286		40.851	12.723	1.00 25.66	A
30	ATOM	1694	N		A 287		40.391	11.239		
50	ATOM	1695	CA		A 287				1.00 24.81	A
•	ATOM	1696	CB		A 287	=	39.662	12.206	1.00 27.59	A
		1697					38.985	11.510	1.00 30.17	A
	ATOM ATOM	1698	CG CD		A 287 A 287		37.632	10.931	1.00 38.21	A
35				GLU Z			36.998	10.140	1.00 41.86	A
33	ATOM	1699 1700					37.036	10.608	1.00 43.08	A
	ATOM		OE2				36.449	9.052	1.00 45.22	A
	ATOM	1701	С		A 287		40.485	13.383	1.00 25.05	A
	ATOM	1702	0		A 287		40.030	14.521	1.00 26.41	A
40	ATOM	1703	N		A 288		41.685	13.122	1.00 23.04	A
40	ATOM	1704	CA		A 288		42.528	14.205	1.00 22.34	A
	MOTA	1705	CB	TYR A			43.913	13.691	1.00 21.07	A
	ATOM	1706	CG		288		44.858	14.805	1.00 21.07	A
	ATOM	1707	CD1			46.533	44.762	15.405	1.00 21.23	A
	ATOM	1708	CE1	TYR A	1 288	46.891	45.588	16.475	1.00 20.43	A
45	MOTA	1709		TYR A			45.809	15.302	1.00 22.32	A
	ATOM	1710		TYR A		•	46.637	16.373	1.00 23.28	A
	MOTA	1711	CZ	TYR A			46.518	16.953	1.00 22.96	Α
	MOTA	1712	OH	TYR A	288	46.316	47.313	18.024	1.00 23.18	A
	ATOM	1713	С	TYR A	288	43.402	42.698	15.288	1.00 21.38	A
50	ATOM	1714	0	TYR A	288	43.710	42.616	16.473	1.00 22.09	A
	MOTA	1715	N	LEU F	289	42.159	42.939	14.874	1.00 21.88	A
	ATOM	1716	CA	LEU F	289	41.055	43.130	15.811	1.00 21.98	A
	ATOM	1717	CB	LEU F	289	39.821	43.673	15.078	1.00 22.90	A
	ATOM	1718	CG	LEU P	289	39.896	45.130	14.601	1.00 26.52	A
55	ATOM	1719		LEU P		38.706	45.436	13.696	1.00 26.55	A
	ATOM	1720		LEU A		39.914	46.071	15.807	1.00 23.13	A
	ATOM	1721	С	LEU A		40.686	41.849	16.560	1.00 21.24	A
	ATOM	1722	Ō	LEU A		40.256	41.897	17.715	1.00 20.72	A
	ATOM	1723	N	ILE A		40.843	40.708	15.900	1.00 19.62	A
										••

	ATOM	1724	CA	ILE F		-	40.538	39.433	16.533	1.00 18.54	А
	ATOM	1725	СB	ILE A			40.560	38.281	15.509	1.00 18.52	A
	ATOM	1726		2 ILE A			40.503	36.934	16.234	1.00 17.63	A
	ATOM	1727	CG:	L ILE A			39.378	38.429	14.545	1.00 18.88	A
5	ATOM	1728	CD:				39.421	37.483	13.357	1.00 19.81	A
	MOTA	1729	.C	ILE A	290		41.578	39.167	17.618	1.00 19.09	· A
	ATOM	. 1730	0	ILE A			41.236	38.788	18.737	1.00 18.20	A
	MOTA	1731	N	PHE A			42.849	39.376	17.286	1.00 18.76	A
	ATOM	1732	CA	PHE A			43.925	39.156.	18.247	1.00 20.75	A
10	MOTA	1733	CB	PHE A			45.286	39.434	17.606	1.00 20.71	A
	ATOM	1734	CG	PHE A			45.644	38.480	16.503	1.00 22.92	A
	MOTA	1735		PHE A			45.065	37.214	16.443	1.00 22.98	A
	ATOM	1736		PHE A			46.588	38.830	15.543	1.00 22.91	A
	MOTA	1737		PHE A			45.423	36.310	15.440	1.00 24.51	A
15	MOTA	1738		PHE A			46.954	37.931	14.535	1.00-25.54	A
	ATOM	1739	CZ	PHE A			46.370	36.670	14.485	1.00 23.29	A
	MOTA	1740	C	PHE A			43.739	40.061	19.451	1.00 21.72	A
	ATOM	1741	0	PHE A			43.992	39.671	20.593	1.00 22.32	A
00	ATOM	1742	N	GLN A			43.284	41.275	19.178	1.00 23.27	A:
20	ATOM	1743	CA	GLN A			43.055	42.264	20.216	1.00 24.01	A
	MOTA	1744	CB	GLN A			42.574	43.559	19.562	1.00 25.77	A
	ATOM	1745	CG	GLN A			42.577	44.773	20.447	1.00 28.45	A
	MOTA	1746	CD	GLN A			42.469	46.057	19.638	1.00 29.83	A
25	ATOM	1747		GLN A			41.520	46.244	18.872	1.00 27.16	A
25	ATOM	1748		GLN A GLN A			43.449	46.944	19.799	1.00 27.61	A
	ATOM ATOM	1749 1750	С 0	GLN A			42.018	41.733	21.204	1.00 22.97	A
	ATOM	1751	Ŋ	LYS A			42.200 40.937	41.832	22.415	1.00 21.64	A
	ATOM	1752	CA	LYS A			39.895	41.154 40.612	20.687	1.00 21.82	A
30	ATOM	1753	CB	LYS A			38.664	40.812	21.558 20.740	1.00 22.18 1.00 22.69	A A
50	ATOM	1754	CG	LYS A			37.919	41.407	20.740	1.00 22.89	A A
	ATOM	1755	CD	LYS A			36.651	40.961	19.429	1.00 23.78	A
	ATOM	1756	CE	LYS A			35.857	42.161	18.926	1.00 27.88	A
	ATOM	1757	NZ	LYS A			34.612	41.750	18.214	1.00 32.98	A
35	ATOM	1758	C	LYS A			40.398	39.398	22.343	1.00 21.20	. A
	ATOM	1759	ō	LYS A			40.041	39.204	23.509	1.00 22.01	A
	ATOM	1760	N	ILE A			41.226	38.583	21.702	1.00 19.91	
	ATOM	1761	CA	ILE A	294		41.774	37.394	22.347	1.00 20.28	A
	ATOM	1762	CB	ILE A	294		42.631	36.575	21.349	1.00 18.98	A
40	ATOM	1763	CG2	ILE A	294		43.481	35.550	22.098	1.00 17.70	A
	ATOM	1764	CG1	ILE A	294		41.716	35.897	20.318	1.00 17.93	Α
	ATOM	1765	CD1	ILE A	294		42.467	35.237	19.178	1.00 16.21	A
	MOTA	1766	С	ILE A	294		42.618	37.727	23.587	1.00 21.94	Α
	MOTA	1767	0	ILE A	294		42.366	37.199	24.673	1.00 20.86	Α
45	ATOM	1768	N	ILE A			43.610	38.600	23.439	1.00 21.88	A
	MOTA	1769	CA	ILE A			44.461	38.934	24.582	1.00 24.25	·A
	ATOM	1770	CB	ILE A			45.668	39.805	24.175	1.00 23.93	A
	MOTA	1771		ILE A			46.514	39.066	23.140	1.00 24.61	А
	MOTA	1772		ILE A			45.189	41.151	23.637	1.00 24.58	A
50	ATOM	1773		ILE A			46.317	42.149	23.433	1.00 26.69	Α
	ATOM	1774	C	ILE A			43.720	39.636	25.717	1.00 24.80	A
	ATOM	1775	0	ILE A			44.214	39.687	26.842	1.00 24.76	A
	ATOM	1776	Ŋ	LYS A			42.539	40.173	25.425	1.00 25.33	A
55	ATOM	1777	CA	LYS A			41.743	40.853	26.444	1.00 26.80	A
55	ATOM	1778	CB	LYS A			41.178	42.170	25.894	1.00 27.39	A
	ATOM	1779	CG	LYS A			42.240	43.141	25.413	1.00 31.79	A
	ATOM ATOM	1780 1781	CD	LYS A			41.634	44.410	24.826	1.00 35.56	A
			CE	LYS A			41.009	45.283	25.900	1.00 39.29	A
	ATOM	1782	NZ	пір А	270		40.564	46.603	25.357	1.00 41.72	A

	ATOM	1783	С	LYS	A	296		40.59	93	39.958	26.893	1.00	25.50	A
•	ATOM	1784	0	ĹYS	Α	296		39.77	70	40.361	27.713	1.00	24.02	A
	ATOM	1785	N	LEU	Α	297		40.55	50	38.742	26.349	1.00	25.67	A
	ATOM	1786	CA	LEU	A	297		39.50	00	37.777	26.666	1.00	25.16	A
5	MOTA	1787	CB	LEU	Α	297		39.63	32	37.285	28.111	1.00	24.80	Α
	MOTA	1788	CG	LEU	Α	297		38.76	66	36.068	28.460	1.00	26.43	A
	MOTA	1789	CD1	LEU	A	297	• •	39.23	88	34.852	27.646	1.00	26.70	Α
	ATOM	1790	CD2	LEU	Α	297		38.85	66	35.777	29.951	1.00	24.84	A
	ATOM	1791	С	LEU	A	297		38.15	51	38.459	26.467	1.00	25.11	A
10	ATOM	1792	0	LEU	Α	297		37.26	51	38.378	27.309		25.28	A
	ATOM	1793	N	GLU	Α	298		38.00	7	39.127	25.331	1.00	24.98	A
	ATOM	1794	CA	GLU	Α	298		36.78	36	39.847	25.023	1.00	25.31	. A
	ATOM	1795	CB	GLU	Α	298		37.14	13	41.139	24.291		27.13	A
	ATOM	1796	CG	GLU	A	298		35.99	91	42.092	24.108	1.00	31.28	A
15	MOTA	1797	CD	GLU	A	298		36.41	١9	43.362	23.410		34.40	A
	MOTA	1798	OE1	GLU	Α	298		37.34	18	44.027	23.918		35.90	A
	ATOM	1799	OE2	GLU	A	298		35.83	32	43.693	22.359		36.16	A
	MOTA	1800	С	GLU	A	298		35.76	56	39.057	24.207		23.79	A
	ATOM	1801	0	GLU	Α	298		35.83	32	39.017	22.979		24.35	A
20	MOTA	1802	N	TYR	Α	299		34.82	25	38.427	24.902		23.45	A
	ATOM	1803	CA	TYR	A	299		33.76		37.663	24.265		23.98	A
	MOTA	1804	CB	TYR				34.26		36.304	23.755		20.13	A
	ATOM	1805	CG	TYR				34.34		35.233	24.828		21.17	A
	ATOM	1806	CD1	TYR	A	299		35.33		35.279	25.810		19.32	A
25	MOTA	1807	CEI					35.38		34.332	26.826		19.30	A
	ATOM	1808	CD2	TYR				33.41		34.201	24.888		18.96	A
	MOTA	1809	CE2	TYR				33.45		33.243	25.907		19.41	A
	ATOM	1810	CZ	TYR				34.44		33.321	26.870		18.79	A.
	MOTA	1811	OH	TYR				34.5		32.401	27.881		18.77	A
30	ATOM	1812	С	TYR				32.69		37.437	25.331		25.20	A
	MOTA	1813	0	TYR				32.94		37.681	26.506		26.46	A
	MOTA	1814	N	ASP				31.52		36.981	24.927		26.94	A A
	MOTA	1815	CA	ASP				30.4		36.710	25.891		30.60 35.86	A
	ATOM	1816	CB	ASP				29.66		37.981	26.179		42.04	A
35	MOTA	1817	CG	ASP				29.22		38.687	24.923 24.149	-	45.98	A
	MOTA	1818		ASP				28.45		38.088			45.69	A
	ATOM	1819		ASP				29.60		39.840	24.707 25.363		29.26	A
	MOTA	1820	С	ASP				29.50		35.608 35.299	24.172		28.64	A
4.0	ATOM	1821	0	ASP				29.59		35.011	26.253		28.96	A
40	MOTA	1822	N	PHE				28.7° 27.88		33.924	25.871		30.48	A
	ATOM	1823	CA	PHE				27.83		32.854	26.968		29.17	A
	ATOM	1824	CB	PHE				29.1		32.279	27.356		29.29	A
	ATOM	1825	CG	PHE PHE				29.9		32.949	28.245		27.31	A
15	ATOM	1826						29.5		31.050	26.845		27.89	A
45	ATOM	1827		PHE				31.20		32.403	28.625		28.83	A
	ATOM	1828		PHE PHE				30.78		30.498	27.217		28.05	Α
	ATOM	1829 1830	CEZ	PHE				31.6		31.175	28.110		28.27	Α
	ATOM	1831	C	PHE				26.4		34.384	25.619		32.20	A
50	ATOM	1832	0	PHE				25.9		35.261	26.317		32.36	A
50	ATOM ATOM	1833	N	PRO				25.7		33.804	24.607		33.29	A
	ATOM	1834	CD	PRO				26.3		32.943	23.529		34.04	A
	ATOM	1835	CA			302		24.4		34.199	24.341		35.24	A
	ATOM	1836	CB			302		24.1		33.608	22.959		34.01	Α
55	ATOM	1837	CG			302		25.0		32.413	22.921		35.48	Α
J.J	ATOM	1838	C			302		23.5		33.561	25.444		37.39	A
	ATOM	1839	Ö			302		23.9		32.518	25.986		38.49	A
	ATOM	1840	N			303		22.4		34.188	25.783		39.36	A
	ATOM	1841	CA			303		21.5		33.692	26.843		40.65	A
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	ATOM	1842	СВ	ALA A	303		20.280	34.506	26.862	1.00	41.66	A
•	ATOM	1843	С	ALA A			21.238	32.197	26.814	1.00	41.25	A
	ATOM	1844	0	ALA A			21.253	31.537	27.854		43.16	A
	ATOM	1845	N	ALA A	304		20.945	31.665	25.631		41.04	A
5	ATOM	1846	CA	ALA A	304		20.569	30.258	25.480	1.00	40.66	A
_	ATOM	1847	CB	ALA A			20.121	30.004	24.040	1.00	41.36	Α
	ATOM	1848	С	ALA A			21.628	29.223	25.876		39.61	A
	ATOM	1849	0	ALA A	304		21.298	28.156	26.395	1.00	40.61	A
	ATOM	1850	N	PHE A	305		22.891	29.543	25.617	1.00	36.21	A
10	ATOM	1851	CA	PHE A	305		24.022	28.662	25.909		32.08	A
	ATOM	1852	CB	PHE A	305		25.259	29.519	26.187		29.46	A
	ATOM	1853	CG	PHE A	305		26.536	28.917	25.690		28.15	A
	MOTA	1854	CD1	PHE A	305		27.146	27.875	26.377		26.20	A
	ATOM	1855	CD2	PHE A	305		27.127	29.386	24.521		27.05	A
15	ATOM	1856	CE1	PHE A	305		28.330	27.308	25.908		26.92	· A
	ATOM	1857	CE2	PHE A	305		28.312	28.826	24.042		26.62	A
	ATOM	1858	CZ	PHE A	305		28.914	27.786	24.737		26.61	A
	ATOM	1859	С	PHE A	305		23.811	27.664	27.057		30.09	
	ATOM	1860	0	PHE A	305		23.518	28.051	28.187		31.51	A
20	ATOM	1861	N	PHE A	306		23.964	26.378	26.758		27.01	A
	ATOM	1862	CA	PHE A			23.801	25.334	27.769		26.30	A
	MOTA	1863	CB	PHE A	306		24.157	23.970	27.170		25.03	A
	ATOM	1864	CG	PHE A			23.548	23.725	25.815		27.24	A
	MOTA	1865	CD1	PHE A	306		22.170	23.831	25.622		28.40	A
25	ATOM	1866	CD2	PHE A	306		24.350	23.386	24.728		27.84	A
	ATOM	1867		PHE A			21.601	23.603	24.365		28.05	A
	ATOM	1868	CE2	PHE A			23.792	23.155	23.465		28.31	. A.
	MOTA	1869	CZ	PHE A			22.415	23.263	23.283		28.00	A A
	ATOM	1870	С	PHE A			24.711	25.652	28.961		26.23 25.59	A
30	MOTA	1871	0	PHE A			25.927	25.775	28.811		26.67	A
	MOTA	1872	N	PRO A			24.125	25.796	30.163		27.95	A
	MOTA	1873	CD	PRO A			22.685	25.625	30.430		26.59	A
	MOTA	1874	CA	PRO A			24.842	26.110	31.405		26.14	A
	MOTA	1875	CB	PRO A			23.795	25.832	32.481 31.803		27.86	A
35	MOTA	1876	CG	PRO A			22.531	26.250 25.355	31.659		25.58	A
•	ATOM	1877	Ċ	PRO A			26.145	25.964	31.900		22.65	A
	MOTA	1878	0	PRO A			27.189	24.031	31.620		24.46	A
	MOTA	1879	Й	LYS A			26.085 27.274	23.232	31.867		23.91	A
	ATOM	1880	CA	LYS A			26.887	21.760	32.024		23.25	A
40	ATOM	1881	CB	LYS A			26.062	21.532	33.285		28.49	A
	ATOM	1882	CG	LYS A			25.618	20.093	33.466		30.17	A
	ATOM	1883	CD	LYS A			24.760	19.973	34.722		33.12	А
	ATOM	1884	CE	LYS A			24.122	18.636	34.860		34.13	Α
45	ATOM	1885	NZ	LYS A			28.314	23.426	30.769		22.84	A
45	MOTA	1886	С	LYS A	308		29.514	23.411	31.042		22.46	A
	ATOM	1887	0	ALA A			27.861	23.621	29.534		21.59	A
	ATOM	1888	N CA	ALA A			28.792	23.848	28.432		20.02	A
	MOTA	1889	CB	ALA A			28.056	23.856	27.106		18.80	Α
50	MOTA MOTA	1890 1891	C	ALA A			29.481	25.191	28.662	1.00	21.41	A
50	ATOM	1892	0	ALA A			30.680	25.335	28.427		21.39	Α
	ATOM	1893	N	ARG A			28.717	26.179	29.121	1.00	21.39	A
•	ATOM	1894	CA	ARG A			29.290	27.494	29.388		22.02	Α
		1895	CB	ARG I			28.213	28.479	29.854	1.00	22.39	A
55	ATOM ATOM	1896	CG	ARG A			28.806	29.756	30.436	1.00	25.30	Α
,,	ATOM	1897	CD	ARG A			27.780	30.852	30.664		28.33	Α
	ATOM	1898	NE	ARG A			28.420	32.039	31.230		30.18	A
	ATOM	1899	CZ	ARG A			27.901	33.263	31.203		32.07	A
	ATOM	1900		1 ARG A		_	26.719	33.477	30.634	1.00	31.19	A
	AION	1000	7411.		- -	•						

	ATOM	1901	NH	2 ARG	Α	310	28.5	67	34.2	77	31.742	1.0	30.4	19	А	
	ATOM	1902	C.			310	30.3		27.38		30.458		21.6		A	
	ATOM	1903	0			310	31.4		27.9		30.311		20.3		A	
	MOTA	1904	N	ASP			30.0		26.6		31.541		19.5		A	
5	ATOM	1905	CA	ASP			31.0		26.53		32.615		20.1		A	
	ATOM	1906	СВ	ASP			30.4		25.64		33.739		20.3		A	
	ATOM	1907	CG	ASP			31.4		25.44		34.881		23.3		A	
	ATOM	1908		ASP			32.1		24.42		34.885		24.9	_	A	
	ATOM	1909		ASP			31.5		26.31		35.776		26.9		A	
10	ATOM	1910	Ċ,	ASP			32.3		25.87		32.073		19.7		A	
	ATOM	1911	o	ASP			33.4		26.28		32.439		19.7		A	
	ATOM	1912	N	LEU			32.1		24.89		31.188		16.3		A	
	ATOM	1913	CA	LEU			33.3		24.22		30.611		16.6		A	
	ATOM	1914	СВ	LEU			32.9		23.03		29.744		16.1			
15	ATOM	1915	CG	LEU			34.0		22.32		28.974				A	
	ATOM	1916		LEU			35.1		21.93		29.912		14.7 14.5		A	
	ATOM	1917		LEU			33.4		21.08		28.289		14.2		A	
	ATOM	1918	C	LEU			34.1		25.18		29.774				A	
	ATOM	1919	Ö	LEU			35.4		25.24		29.910		16.6		A	
20	ATOM	1920	N	VAL			33.5		25.24		28.908		16.2		A	
	ATOM	1921	CA	VAL			34.2		26.90				16.2		A	
	ATOM	1922	CB	VAL			33.2		27.64		28.058		15.3		A	
	ATOM	1923		VAL			33.9		28.79		27.130 26.426		16.4		A	
	ATOM	1924		VAL			32.6		26.67		26.103		16.9		A	
25	ATOM	1925	C	VAL			34.9		27.92		28.911		17.8		A	
	ATOM	1926	Ö	VAL			36.0		28.29		28.591		17.3 18.0		A	
	ATOM	1927	N	GLU			34.3		28.36		30.004			-	A	
	ATOM	1928	CA	GLU			34.9		29.33		30.885		17.6		A	
	ATOM	1929	CB	GLU			34.0		29.81		31.959		20.4		A	
30	ATOM	1930	CG	GLU			32.8		30.55		31.396		22.1		A	
	ATOM	1931	CD	GLU			31.8		31.02				26.5		A	
	ATOM	1932		GLU			31.5		30.24		32.478 33.417		31.2		A	
	ATOM	1933		GLU			31.3		32.17		32.387		33.4		A	
	ATOM	1934	C	GLU			36.2		28.72		32.307		34.8		A	
35	ATOM	1935	Ö	GLU			37.13		29.43		31.934		19.15 21.4		A	
	ATOM	1936	N	LYS			36.2		27.40						A	
	ATOM	1937	CA	LYS			37.39		26.74		31.651 32.258		19.5		A	
	ATOM	1938	CB	LYS			36.9		25.51				19.17		A	
	ATOM	1939	CG	LYS			36.28		25.88		33.043 34.368		18.84		A	
40	ATOM	1940	CD	LYS			35.65		24.69				19.62		A	
	ATOM	1941	CE	LYS		315	35.07		25.09		35.073		19.22		A	-
	ATOM	1942	NZ	LYS		315	36.11		25.55		36.427 37.381		19.53		AC:	
	ATOM	1943	C	LYS			38.45		26.39		31.218		18.96		AC:	T
	ATOM	1944	Ö	LYS			39.51		25.87		31.561				A	
45	ATOM	1945	N	LEU									19.85		A	
	ATOM	1946	CA	LEU			38.16		26.693 26.429		29.950		17.08		Α	
	ATOM	1947	CB	LEU			38.41		25.63		28.854 27.738		16.41		Α.	
	ATOM	1948	CG	LEU			38.02		24.20				13.81		A	
	ATOM	1949		LEU	д Э 2	16	37.13		23.59		28.115 27.031		14.39		A	
50	ATOM	1950		LEU			39.30		23.37		28.309				A	
-	ATOM	1951	C	LEU			39.65						12.77		A	
	ATOM	1952	0	LEU			40.85		27.743 27.860		28.290		17.12		A	
	ATOM	1953	N	LEU			38.78				28.023		16.53		A	
	ATOM	1954	CA	LEU			39.22		28.729		28.105		16.27		A	
55	ATOM	1955	CB	LEU			38.08		30.022		27.596		17.52		A	
	ATOM	1956	CG	LEU .			37.44		30.752		26.887		16.37		A	
	ATOM	1957		LEU .			36.41		29.973		25.727		18.81		A	
	ATOM	1958		LEU .					30.851		25.018		16.47		A	
	ATOM	1959	CD2				38.52		29.526		24.741		17.87		A	
	WY OLI	1933	C	LEU .	n)	1 . /	39.74	3	30.841	T 2	28.774	T.00	18.27		Α	

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	ATOM	1960	0	LEU	Α	317		39.	078	31.753	29.	273	1.00	18.58	3 A	L
	ATOM	1961	N	VAL	A	318		40.	937	30.475		229	1.00	18.02	2 A	
	MOTA	1962	CA	VAL	Α	318		41.	593	31.141	30.	342	1.00	18.85	5 А	L.
	ATOM	1963	СВ	VAL	Α	318		41.	846	30.153	31.	500	1.00	19.91	. А	L
5	MOTA	1964		VAL				42.	590	30.848	32.	634	1.00	20.01	. А	<u>k</u>
	MOTA	1965	CG2	VAL				40.	520	29.584	31.		1.00	19.44	l A	L
	MOTA	1966	С	VAL	Α	318	•	42.	923	31.657	29.	811	1.00	19.67	A	į.
	MOTA	1967	0	VAL	Α	318		43.	690	30.902	29.	208	1.00	18.26	5 A	L
	ATOM	1968	N	LEU	Α	319		43.	197	32.939	30.	028	1.00	20.07	A	L
10	ATOM	1969	CA	LEU	А	319		44.	436	33.533	29.	538	1.00	20.98	A	L
	MOTA	1970	CB	LEU	Α	319	•	44.	521	35.002	29.	968	1.00	21.64	A	L
	MOTA	1971	CG	LEU	А	319		43.	418	35.908	29.	408	1.00	24.38	A	
	MOTA	1972	CD1	LEU	Α	319		43.	606	37.332	29.	935	1.00	23.28	A	
	ATOM	1973	CD2	LEU	А	319		43.	453	35.887	27.	875	1.00	24.33	A	
15	MOTA	1974	, C	LEU	A	319		45.	680	32.774	29.	994	1.00	20.38	A	
	ATOM	1975	0	LEU	Α	319		46.	568	32.496	29.	192		21.34		
	ATOM	1976	N	ASP	Α	320		45.	742	32.440	31.	280	1.00	20.22	A	
	ATOM	1977	CA	ASP	A	320		46.	879	31.707	31.	833		20.90		
	ATOM	1978	CB	ASP	Α	320		46.	842	31.760	33.			20.76		
20	MOTA	1979	CG	ASP				48.	049	31.102	34.			21.51		
	ATOM	1980	OD1	ASP	Α	320		48.	669	30.226	33.	367		23.46		
	ATOM	1981	OD2	ASP				48.	371	31.450	35.		1.00	23.89		
	MOTA	1982	С	ASP					814	30.247	31.			20.06		
	ATOM	1983	0	ASP	Α	320		45.	988	29.476	31.			20.54		
25	MOTA	1984	N	ALA					700	29.876	30.			20.68		
	MOTA	1985	CA	ALA					733	28.522	29.			22.04		
	MOTA	1986	CB	ALA				48.	860	28.411	28.			20.75		
	MOTA	1987	С	ALA				47.	858	27.400	30.			21.62		
	MOTA	1988	0	ALA					482	26.259	30.			21.99		
30	ATOM	1989	N	THR					372	27.715	32.			20.89		
	MOTA	1990	CA	THR					531	26.698	33.			20.82		
	MOTA	1991	CB	THR					670	27.051	34.			19.47		
	MOTA	1992	OG1	THR					341	28.253	34.			20.19		
	MOTA	1993	CG2	THR					981	27.249	33.			21.59		
35	MOTA	1994	С	THR					264	26.498	33.			19.55		
	ATOM	1995	0	THR					235	25.673	34.			21.13		
	ATOM	1996	N	LYS					216	27.248	33.			19.33		
	ATOM	1997	CA	LYS					962	27.122	34.			21.20		
4.0	ATOM	1998	CB	LYS					580	28.460	35.			23.75		
40	MOTA	1999	CG	LYS					562	28.933	36.			28.45		
	ATOM	2000	CD	LYS					055	30.177	36.			33.76		
	ATOM	2001	CE	LYS					087	30.678	37.			36.15		
	ATOM	2002	NZ	LYS					532	29.569	33.	693°) 37.34) 20.68		
45	ATOM	2003	C	LYS					806	26.614						
45	ATOM	2004	0	LYS					649	26.757	33.			.20.42		
	ATOM	2005	N	ARG					114	26.019	32.			19.97		
	ATOM	2006	CA	ARG					060	25.494	31.) 17.98) 15.95		
	ATOM	2007	CB	ARG					461	25.609	30.					
50	ATOM	2008	CG	ARG				43.		27.050	29.			17.34		
50	ATOM	2009	CD	ARG					996	27.194	28.) 19.80) 16.93		
	ATOM	2010	NE	ARG				44.		28.565	27.					
	ATOM	2011	CZ	ARG				45.		28.908	27.) 19.88) 14.58		
	ATOM	2012		ARG				46.		27.978	26. 27.			16.51		
E	ATOM	2013		ARG				45.		30.181	31.			18.32		
55	ATOM	2014	C	ARG				42.		24.046				18.32		
	ATOM	2015	O N	ARG					673 479	23.222	32. 32.			18.20		
	ATOM	2016	N	LEU					479	23.748				17.79		
	ATOM	2017	CA	LEU					050	22.403	32.			17.03		
	ATOM	2018	СВ	LEU	М	343		J9.	523	22.335	32.	440	1.00	, 17.03	, А	

	ATOM	2019	CG	LEU .	A :	325	38.896	21.125	33.116	1.00	15.91	A
	ATOM	2020	CD1	LEU .			39.392	21.048	34.557		15.93	Ά
		2021						21.255	33.084			
	ATOM			LEU			37.375				16.56	A
	MOTA	2022	С	LEU .	A :	325	41.599	21.433	31.356	1.00	18.68	Α
5	ATOM	2023	0	LEU .	Α:	325	41.347	21.586	30.157	1.00	18.28	Α
	ATOM	2024	N	GLY .			42.354	20.439	31.821		18.18	A
							42.931	19.462				
	ATOM	2025	CA	GLY .					30.915		16.36	A
	ATOM	2026	С	GLY .	Α:	326	44.443	19.558	30.807	1.00	19.15	Α
	ATOM	2027	0	GLY .	A :	326	45.093	18.592	30.404	1.00	19.52	Α
10	ATOM	2028	N	CYS			45.016	20.708	31.161		18.16	A
10								20.867	31.075		19.30	
	MOTA	2029	CA	CYS			46.463					Α
	ATOM	2030	CB	CYS .	Α.	327	46.856	22.350	31.058	1.00	20.22	Α
	ATOM	2031	SG	CYS .	A :	327	46.782	23.200	32.649	1.00	21.97	A
	ATOM	2032	С	CYS	Δ 1	327	47.169	20.157	32.228	1.00	20.22	Α
1.5		2033					46.561	19.828	33.246		17.92	A
15	ATOM		0	CYS								
	ATOM	2034	И.	GLU Z			48.463	19.933	32.053		20.51	A
	MOTA	2035	CA	GLU 2	A 3	328	49.274	19.244	33.042	1.00	23.34	A
	ATOM	2036	CB	GLU Z	A 3	328	50.710	19.139	32.507	1.00	28.68	Α
	ATOM	2037	CG	GLU I			50.754	18.367	31.175		38.24	A
20								18.500			43.23	
20	ATOM	2038	CD	GLU 1			52.067		30.414			A
	ATOM	2039		GLU Z			52.535	19.643	30.218		46.22	A
	MOTA	2040	OE2	GLU Z	A 3	328	52.618	17.459	29.991	1.00	44.90	A
	ATOM	2041	С	GLU Z			49.234	19.876	34.435	1.00	22.11	A
	ATOM	2042	Ö	GLU Z			49.147	19.161	35.437		20.27	A
~-												
25	MOTA	2043	N	GLU I			49.276	21.204	34.506		18.40	A
	ATOM	2044	CA	GLU 2	A 3	329	49.248	21.875	35.801	1.00	20.13	A
	ATOM	2045	CB	GLU :	A 3	329	49.587	23.363	35.657	1.00	20.36	A
	ATOM	2046	CG	GLU 2	Α 1	329	51.014	23.651	35.190	1.00	24.05	A
		2047	CD	GLU I			51.191	23.518	33.688		25.93	A
	ATOM											
30	ATOM	2048		GLU			50.213	23.154	32.995		26.61	A
	ATOM	2049	OE2	GLU :	4 :	329	52.311	23.781	33.198	1.00	27.19	A
	ATOM	2050	С	GLU 2	A :	329	47.890	21.718	36.480	1.00	19.36	A
	ATOM	2051	0	GLU :			47.775	21.879	37.694	1.00	18.74	Α.
	ATOM	2052	N	MET .			46.863.	21.415	35.691		17.28	A
26								21.220	36.229		16.38	A
35	MOTA	2053	CA	MET .			45.520					
	ATOM	2054	CB	MET .	Α :	330	44.474	21.833	35.294		17.65	A
	ATOM	2055	CG	MET 2	Α :	330	44.460	23,365	35.311	1.00	22.95	A
	ATOM	2056	SD	MET .	A :	330	44.186	24.026	36.979	1.00	26.78	A
	ATOM	2057	CE	MET			42.435	23.712	37.186	1.00	24.69	A
40				MET :			45.257	19.730	36.422		14.30	A
40	MOTA	2058	C									
	ATOM	2059	0	MET 2			44.127	19.304	36.629		15.39	A
	ATOM	2060	N	GLU 2	A :	331	46.327	18.949	36.346		15.60	A
	ATOM	2061	CA	GLU .	A :	331	46.289	17.501	36.531	1.00	17.08	· A
	ATOM	2062	СВ	GLU I	Δ :	331	45.607	17.155	37.862	1.00	17.00	Α
15									39.038		17.46	A
45	ATOM	2063	CG	GLU A			46.070	18.027				
	ATOM	2064	CD	GLU Z			47.591	18.179	39.145		20.16	A
	ATOM	2065	OE1	GLU	A :	331	48.034	19.073	39.896	1.00	21.39	A
	MOTA	2066	OE2	GLU Z	A 3	331	48.345	17.420	38.500	1.00	18.87	A
	ATOM	2067	C	GLU 2			45.697	16.658	35.398		17.80	A
											20.40	A
50	MOTA	2068	0	GLU I			45.107	15.602	35.636			
	MOTA	2069	N	GLY 2	A 3	332	45.844	17.133	34.167		16.23	A
	MOTA	2070	CA	GLY 2	A :	332	45.420	16.353	33.015	1.00	14.10	A
	ATOM	2071	С	GLY A			43.982	16.154	32.596	1.00	13.54	A
				GLY :			43.063	16.864	33.017		11.96	A
	ATOM	2072	0								14.37	A
55	MOTA	2073	N	TYR A			43.804	15.141	31.750			
	MOTA	2074	CA	TYR Z	4 3	333	42.510	14.806	31.182		13.56	A
	ATOM	2075	CB	TYR Z	A 3	333	42.722	13.892	29.968		15.00	Α
	ATOM	2076	CG	TYR			43.153	14.683	28.752	1.00	16.46	A
	ATOM	2077		TYR			42.206	15.172	27.849		15.29	A
	VIOL	2011	CDI	110		JJJ	12.200	12				

	ATOM	2078	CE1	TYR	Δ	333	42.573	16.002	26.794	1 00	13.42	A
									_			
	ATOM	2079	CD2	TYR			44.490	15.039	28.561	1.00	14.91	Α
	ATOM	2080	CE2	TYR	Α	333	44.872	15.877	27.499	1.00	14.87	Α
	ATOM	2081	CZ	TYR			43.902	16.353	26.626		15.61	A
_												
5	ATOM	2082	ОН	TYR	A	333	44.244	17.197	25.599	1.00	17.29	A
	ATOM	2083	С	TYR	Α	333	41.470	14.230	32.127	1.00	15.23	A
•	ATOM	2084	0	TYR			40.278	14.323	31.846	1.00	16.63	A
	ATOM	2085	N	GLY	A	334	41.907	13.650	33.244	1.00	15.50	A
	ATOM	2086	CA	GLY	Δ	334	40.957	13.100	34.202	1 00	15.07	A
10												
10	ATOM	2087	С	GLY .	A	334	39.925	14.146	34.616	1.00	16.40	A
	ATOM	2088	0	GLY .	Α	334	38.724	13.946	34.433	1.00	15.05	A
	ATOM	2089	N	PRO .			40.366	15.278	35.184		14.96	
	ATOM	2090	CD	PRO .	Α	335	41.727	15.531	35.689	1.00	15.88	A
	ATOM	2091	CA	PRO .	Α	335	39.444	16.339	35.606	1.00	15.29	Α
1.5							•					
15	ATOM	2092	CB	PRO .			40.383	17.397	36.178		13.19	A
	ATOM	2093	CG	PRO .	A	335	41.485	16.569	36.758	1.00	13.81	Α
	ATOM	2094	С	PRO .	Δ	335	38.594	16.877	34.448	1 00	15.84	A
						•						
	ATOM	2095	0	PRO .	А	335	37.423	17.204	-34.631		14.84	Α
	ATOM	2096	N	LEU .	Α	336	39.184	16.971	33.257	1.00	16.12	A
20	ATOM	2097	CA	LEU .			38.450	17.465	32.094		15.52	A
20												
	ATOM	2098	CB '	LEU .	Α	336	39.396	17.653	30.898	1.00	14.39	A
	ATOM	2099	CG	LEU .	Α	336	38.770	17.991	29.538	1.00	15.46	Α
				LEU			37.836	19.182	29.662		11.25	A
	ATOM	2100										
	ATOM	2101	CD2	LEU .	Α	336	39.884	18.285	28.528	1.00	14.11	A
25	ATOM	2102	С	LEU .	А	336	37.321	16.508	31.714	1.00	16.28	Α
23											15.51	A
	ATOM	2103	O.	LEU .			36.176	16.921	31.540			
	ATOM	2104	N	LYS .	Α	337	37.640	15.225	31.592	1.00	17.22	A
	MOTA	2105	CA	LYS .			36.624	14.243	31.235	1.00	17.39	A
	ATOM	2106	CB	LYS			37.293	12.900	30.921		17.68	A
30	ATOM	2107	CG	LYS .	Α	337	38.170	12.994	29.676	1.00	22.31	Α
	ATOM	2108	CD	LYS .	Δ	337	39.213	11.892	29.592	1.00	24.60	Α
	MOTA	2109	CE	LYS .			38.620	10.560	29.189		24.76	A
	ATOM	2110	NZ	LYS .	Α	337	39.710	9.560	28.997	1.00	25.05	Α
	ATOM	2111	C .	LYS			35.577	14.096	32.342	1 00	17.33	A
35	ATOM	2112	0	LYS	A	337	34.456	13.652	32.090		14.42	A
	ATOM	2113	N	ALA .	Α	338	35.928	14.500	33.559	1.00	15.83	Α
			CA	ALA			34.989	14.395	34.674	1 00	17.52	A
	ATOM	2114										
	MOTA	2115	CB	ALA	A	338	35.749	14.167	35.980		19.68	A
	ATOM	2116	С	ALA .	Α	338	34.095	15.621	34.804	1.00	18.83	Α
40							33.252	15.687	35.695	1 00	18.94	A
40	ATOM	2117	0	ALA .								
	ATOM	2118	N	HIS .	Α	339	34.262	16.596	33.918	1.00	19.42	A
	ATOM	2119	CA	HIS .	Α	339	33.438	17.796	34.004	1.00	19.28	A
•				HIS			33.865	18.819	32.949	1 00	19.20	Α
	ATOM	2120	CB									
	ATOM	2121	ĊG	HIS .	Α	339	33.163	20.134	33.074		20.26	A
45	ATOM	2122	CD2	HIS .	Δ	339	33.549	21.299	33.649	1.00	18.95	A
15								20.340	32.612		19.10	Α
	ATOM	2123		HIS .			31.880					
	ATOM	2124	CE1	HIS .	Α	339	31.506	21.576	32.896	1.00	22.19	A
	MOTA	2125		HIS .			32.500	22.179	33.525	1.00	21.98	A
•									33.845		19.13	
	ATOM	2126	С	HIS .			31.957	17.448				A
50	ATOM	2127	0	HIS .	Α	339	31.597	16.576	33.061	1.00	19.52	A
- '	ATOM	2128	N	PRO .			31.079	18.125	34.606	1.00	19.80	A
	MOTA	2129	CD	PRO .	А	340	31.424	19.119	35.640		19.08	A
	ATOM	2130	CA	PRO .	Α	340	29.630	17.900	34.569	1.00	20.52	A
	ATOM	2131	CB	PRO			29.091	19.058	35.396		20.74	A
55	MOŢA	2132	CG	PRO .			30.146	19.207	36.454		19.20	A
	ATOM	2133	С	PRO .	Α	340	29.000	17.834	33.176	1.00	21.42	A
	ATOM	2134	Ō	PRO			28.049	17.088	32.955	1.00	22.48	Α
	ATOM	2135	N	PHE .	Α	341	29.528	18.606	32.237		21.33	A
	MOTA	2136	CA	PHE .	А	341	28.985	18.610	30.886	1.00	21.57	A
					-							

	ATOM	2137	CB	PHE A	341	29.739	19.624	30.017	1.00 21.64	А
	ATOM	2138	CG	PHE A		29.207	19.740	28.613		
	ATOM	2139		PHE A		27.903	20.171			· A
	ATOM	2140		PHE A		30.013		28.382	1.00 22.58	A
5	ATOM	2141		PHE A			19.431	27.522	1.00 21.95	A
,						27.410		27.082	1.00 23.54	A
	ATOM	2142		PHE A		29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	CZ	PHE A		28.228	19.980	25.998	1.00 23.23	Α
	ATOM	2144	С	PHE A		29.055	17.226	30.237	1.00 21.84	A
	ATOM	2145	0	PHE A	341	28.232	16.896	29.389	1.00 20.37	Α
10	ATOM	2146	N	PHE A	342	30.034	16.422	30.640	1.00 20.51	A
	ATOM	2147	CA	PHE A	342	30.221	15.085	30.077	1.00 23.01	A
	ATOM	2148	CB	PHE A	342	31.710	14.809	29.850	1.00 18.00	A
	ATOM	2149	CG	PHE A	342	32.398	15.812	28.971	1.00 17.05	A
	MOTA	2150		PHE A		32.010	15.987	27.652	1.00 17.05	A
15	ATOM	2151		PHE A		33.487	16.534	29.450		
	ATOM	2152		PHE A		32.702			1.00 15.72	A
	ATOM	2153		PHE A		34.184	16.867	26.811	1.00 18.08	A
	ATOM	2154		PHE A			17.414	28.617	1.00 17.45	A
						33.790	17.578	27.298	1.00 16.56	Α
20	MOTA	2155		PHE A		29.679	13.972	30.976	1.00 24.95	A
20	MOTA	2156		PHE A		30.002	12.798	30.777	1.00 23.95	A
	ATOM	2157		GLU A		28.861	14.333	31.958	1.00 27.35	A
	MOTA	2158		GLU A		28.325	13.349	32.897	1.00 30.28	A
	MOTA	2159		GLU A		27.187	13.964	33.716	1.00 32.20	A
	ATOM	2160	CG	GLU A	343	26.581	12.991	34.714	1.00 39.71	A
25	ATOM	2161	CD	GLU A	343	25.628	13.661	35.688	1.00 44.72	A
	MOTA	2162	OE1	GLU A	343	24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2	GLU A	343	25.847	13.526	36.911	1.00 46.89	A
	MOTA	2164	С	GLU A	343	27.852	12.017	32.305	1.00 28.98	A
	ATOM	2165	0	GLU A	343	28.225	10.952	32.800	1.00 31.73	A
30	MOTA	2166		SER A		27.037	12.067	31.258	1.00 26.09	A
	ATOM	2167		SER A		26.520	10.838	30.656	1.00 28.36	A
	ATOM	2168		SER A		25.129	11.089	30.067	1.00 28.73	A
	ATOM	2169		SER A		25.203	11.942	28.940	1.00 20.75	· A
	ATOM	2170		SER A		27.407	10.214	29.577	1.00 27.66	A
35	ATOM	2171		SER A		26.987	9.281	28.900	1.00 27.00	
	ATOM	2172		VAL A		28.627	10.715			A
	ATOM	2173		VAL A		29.534		29.419	1.00 26.75	A
	ATOM	2174		VAL A			10.183	28.402	1.00 23.44	A
	ATOM	2175		VAL A		30.565	11.256	27.950	1.00 23.10	A
40				VAL A		31.589	10.631	26.995	1.00 22.24	A
40	MOTA	2176				29.854	12.418	27.275.		Α
	MOTA	2177		VAL A		30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178		VAL A		30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179		THR A		30.374	7.942	27.997	1.00 21.77	A
	ATOM	2180		THR A		31.153	6.740	28.272	1.00 23.70	A
45	ATOM	2181		THR A		30.391	5.455	27.857	1.00 26.53	A
	ATOM	2182		THR A		29.248	5.284	28.706	1.00 29.98	A
	MOTA	2183	CG2	THR A	346 .	31.289	4.231	27.990	1.00 24.28	A
	ATOM	2184	C 1	THR A	346	32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	0 1	CHR A	346	32.306	6.827	26.160	1.00 24.50	А
50	ATOM	2186	N I	TRP A	347	33.508	7.270	28.013	1.00 22.98	A
	ATOM	2187		CRP A		34.744	7.569	27.300	1.00 23.81	A
	ATOM	2188		rrp A		35.683	8.352	28.219	1.00 22.54	A
	ATOM	2189		TRP A		35.128	9.658	28.693	1.00 20.61	A
	ATOM	2190		RP A		35.257	10.927	28.040	1.00 20.01	A
55	ATOM	2191		RP A 3		34.581	11.881	28.838	1.00 19.11	A
	ATOM	2192		RP A 3		35.878	11.351	26.858		
	ATOM	2193		RP A 3		34.397			1.00 18.16 1.00 18.35	A
	ATOM	2193		RP A 3			9.883	29.828		A
	ATOM	2194				34.065	11.218	29.923	1.00 19.51	A
	VIOU	2133	C42 1	RP A 3	74 /	34.510	13.234	28.491	1.00 16.88	A

	ATOM	2196	CZ3	TRP	A 347	35.808	12.701	26.511	1.00 17.23	A
	ATOM	2197	CH2	TRP	A 347	35.127	13.624	27.327	1.00 18.16	A
	ATOM	2198	С	TRP	A 347	35.538	6.429	26.675	1.00 25.79	A
	ATOM	2199	0	TRP .	A 347	36.304	6.654	25.742	1.00 24.67	A
5	ATOM	2200	N	ALA	A 348	35.360	5.215	27.183	1.00 27.10	A
	ATOM	2201	CA	ALA I	A 348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	CB	ALA A	A 348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	С	ALA A	A 348	35.895	3.620	25.256	1.00 27.18	A
	ATOM	2204	0	ALA Z	A 348	36.830	3.148	24.613	1.00 29.41	A
10	ATOM	2205	N	ASN Z	A 349	34.682	3.769	24.735	1.00 26.55	Α
	ATOM	2206	CA		A 349	34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN Z		33.700	1.962	23.444	1.00 29.37	A
	ATOM	2208	CG		A 349	32.299	2.088	24.013	1.00 30.92	A
	MOTA	2209		ASN A		32.045	2.942	24.859	1.00 30.17	A
15	MOTA	2210		ASN A		31.386	1.237	23.553	1.00 33.52	A
	MOTA	2211	С	ASN A		33.599	4.265	22.509	1.00 26.47	A
	ATOM	2212	0		A 349	32.669	3.843	21.819	1.00 25.87	A
	MOTA	2213	N	LEU Z		33.947	5.543	22.518	1.00 24.45	A
	MOTA	2214	CA	LEU A		33.203	6.510	21.721	1.00 23.14	A
20	ATOM	2215	CB	LEU Z		33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU Z		33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217		LEU A		34.646	9.756	23.293	1.00 19.36	A
	MOTA	2218		LEU A		32.220	9.094	23.319	1.00 18.78	A
	ATOM	2219	C	LEU A		33.082	6.152	20.240	1.00 22.60	A
25	ATOM	2220	0	LEU A		32.011	6.296	19.650	1.00 21.15	A A
	ATOM	. 2221	N	HIS A		34.165	5.689	19.627	1.00 23.13 1.00 27.83	A
	ATOM	2222	CA	HIS A		34.089	5.387 5.325	18.204 17.596	1.00 27.83	A
	ATOM	2223	CB	HIS A		35.506 36.082	3.950	17.396	1.00 29.30	A
20	ATOM	2224	CG	HIS A		36.611	3.128	18.431	1.00 32.39	Ā
30	MOTA	2225		HIS A		36.197	3.285	16.291	1.00 32.33	A
	ATOM	2226 2227		HIS A		36.775	2.113	16.493	1.00 33.58	A
	ATOM	2227		HIS A		37.036	1.992	17.782	1.00 33.30	A
	ATOM	2229	C		A 351		4.144	17.874	1.00 28.12	A
35	ATOM ATOM	2230	0		A 351	33.015	3.847	16.707	1.00 29.49	A
33	ATOM	2231	N	GLN A		32.800	3.442	18.908	1.00 29.28	A
	ATOM	2232	CA	GLN A		31.963	2.255	18.726	1.00 29.67	A
	MOTA	2233	CB	GLN .	352	32.366	1.145	19.694	0.50 30.56	AC1
	ATOM	2234	CG	GLN	352	33.169	0.041	19.041	0.50 30.88	AC1
40	ATOM	2235	CD	GLN	352	34.493	-0.186	19.729	0.50 31.21	AC1
	ATOM	2236	OE1		352	34.541	-0.450	20.928	0.50 30.76	AC1
	ATOM	2237	NE2	GLN	352	35.578	-0.084	18.971	0.50 32.30	AC1
	ATOM	2238	С	GLN Z	352	30.504	2.638	18.963	1.00 30.42	Α
	ATOM	2239	0	GLN A	352	29.595	1.831	18.770	1.00 29.01	A
45	ATOM	2240	N	GLN A	A 353	30.290	3.875	19.397	1.00 27.64	Α
	ATOM	2241	CA		353	28.948	4.365	19.652	1.00 27.42	A
	MOTA	2242	CB		353	28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG	GLN A	¥ 353	29.408	4.837	22.115	1.00 27.34	A
•	ATOM	2244	CD	GLN Z	353	29.638	5.914	23.156	1.00 27.19	A
50	ATOM	2245	OE1	GLN A	353	28.875	6.872	23.252	1.00 28.29	A
	ATOM	2246	NE2	GLN A	353	30.687	5.753	23.951	1.00 28.79	A
	ATOM	2247	С	GLN A		28.375	4.989	18.385	1.00 29.00	A
	MOTA	2248	Ο.	GLN A		29.118	5.455	17.516	1.00 29.14	. A
	ATOM	2249	N	THR A		27.053	4.984	18.276	1.00 27.31	A
55	MOTA	2250	CA	THR A		26.390	5.568	17.119	1.00 27.85	A
	MOTA	2251	CB	THR A		24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.07	A
	MOTA	2253		THR A		24.289	5.585	15.709	1.00 29.58	A
	MOTA	2254	С	THR A	A 354	26.244	7.062	17.376	1.00 26.85	A

	ATOM	2255	0	THR	Α	354		25.592	7.475	18.329	1.00 25.	77	A
	ATOM	2256	N			355		26.867	7.898	16.533	1.00 27.		A
	ATOM	2257	CD			355		27.792	7.588	15.431	1.00 25.		A
_	ATOM	2258	CA			355		26.763	9.346	16.734	1.00 27.		. A
5 .	ATOM	2259	CB			355		27.625	9.915	15.609	1.00 24.		A
	ATOM	2260	CG	PRO	Α	355		28.643	8.838	15.385	1.00 25.	54	A
	ATOM	2261	С	PRO	Α	355		25.322	9.837	16.641	1.00 28.	07	A
	ATOM	2262	0	PRO	Α	355		24.548	9.364	15.810	1.00 27.3	24	A
	ATOM	2263	N	PRO	Α	356		24.941	10.792	17.500	1.00 28.3	28	A
10	MOTA	2264	CD	PRO	А	356		25.752	11.560	18.462	1.00 28.3		Α
	ATOM	2265	CA	PRO				23.572	11.306	17.448	1.00 28.		A
	ATOM	2266	СВ	PRO				23.539	12.301	18.604	1.00 28.3		A
	ATOM	2267,	CG	PRO				24.946	12.832	18.612	1.00 26.8		A
1.5	ATOM	2268	C	PRO				23.363	11.978	16.097	1.00 29.2		A
15		2269	0	PRO				24.304	12.537	15.529	1.00 27.2		A
	ATOM	2270	N	ALA				22.143	11.910	15.575	1.00 30.4	45	A
	ATOM	2271	CA	ALA	Α	357		21.848	12.521	14.287	1,00 32.8	81	Α
	ATOM	2272	CB	ALA	Α	357		20.507	12.019	13.757	1.00 31.9	99	Α
	ATOM	2273	С	ALA	Α	357		21.824	14.035	14.448	1.00 35.0	05	A
20	ATOM	2274	0	ALA	Α	357		21.194	14.561	15.369	1.00 35.0	04	Α
	ATOM	2275	N	LEU				22.516	14.730	13.552	1.00 37.8		A
	ATOM	2276	CA	LEU				22.578	16.185	13.597	1.00 42.3		A
	ATOM	2277	CB	LEU				23.679	16.681	12.658	1.00 39.5		A
	ATOM	2278	CG	LEU				25.086	16.285	13.109	1.00 39.5		A
0.5											1.00 39.2		
25	MOTA	2279		LEU				26.102	16.686	12.062			A
	MOTA	2280		LEU				25.395	16.953	14.445	1.00 40.0		A
	MOTA	2281	С			358		21.241	16.837	13.242	1.00 45.9		A
	ATOM	2282	0	LEU				20.874	16.927	12.069	1.00 45.		Α.
	MOTA	2283	N	THR	Α	359		20.530	17.290	14.275	1.00 50.0)6	A
30	ATOM	2284	CA	THR	Α	359		19.223	17.939	14.140	1.00 53.	73	Α
	ATOM	2285	CB	THR	Α	359		19.353	19.428	13.726	1.00 54.0)4	A
	MOTA	2286	OG1	THR				19.995	19.521	12.448	1.00 56.3	35	Α
	ATOM	2287		THR				20.158	20.204	14.763	1.00 54.3	32	A
	MOTA	2288	С	THR			٠	18.309	17.236	13.139	1.00 54.4		A
35	ATOM	2289	Ö	THR				18.483	16.016	12.930	1.00 55.9		Α
23	ATOM	2290		THR				17.407	17.908	12.595	1.00 56.9		A
•				TIP		1		42.566	19.118	34.302	1.00 15.0		s
	ATOM	2291							32.378	19.857	1.00 15.8		s
	MOTA	2292		TIP		2		41.052					s
	MOTA	2293		TIP		3		37.014	33.030	17.747	1.00 16.9		
40	MOTA	2294		TIP		5		45.353	24.370	18.152	1.00 16.8		s
	ATOM	2295		TIP	S	6		31.896	13.930	33.235	1.00 20.4		S
	ATOM	2296			S	7		50.351	22.781	28.249	1.00 21.3		S
	ATOM	2297	OH2	TIP	S	8		45.246	-0.589	-0.734	1.00 17.7	74	S
	ATOM	2298	OH2	TIP	S	11		46.249	-0.348	-8.523	1.00 21.3		S
45	MOTA	2299	OH2	TIP	s	14		45.756	11.148	29.680	1.00 21.9	94	S
	ATOM	2300		TIP		15		44.273	13.157	34.592	1.00 15.6	61	S
	ATOM	2301		TIP		17		53.598	3.722	-1.720	1.00 21.4		S
	ATOM	2302		TIP		18		46.049	13.087	31.565	1.00 20.3		s
	ATOM	2302		TIP		19		53.422	22.401	-3.280	1.00 23.2		S
F0 .										5.383	1.00 22.5		s
50	ATOM	2304		TIP		20		34.587	7.922				
	ATOM	2305		TIP.		21		45.053	27.379	19.376	1.00 29.6		S
	ATOM.	2306		TIP		23		28.899	36.416	28.633	1.00 31.6		S
	ATOM	2307		TIP		24		35.531	11.645	-8.219	1.00 23.4		S
	ATOM	2308		TIP		25		47.364	28.787	19.612	1.00 23.0		S
55	MOTA	2309	OH2	TIP	S	27		48.859	21.588	12.634	1.00 23.7		S
	MOTA	2310	OH2	TIP	S	29		48.805	8.920	23.626	1.00 22.2		S
	ATOM	2311	OH2	TIP	S	31		48.619	7.247	10.112	1.00 21.3		S
	ATOM	2312		TIP		34		44.824	28.720	15.621	1.00 25.2		s
	ATOM	2313		TIP		35		26.030	12.634	13.407	1.00 21.6		S

	MOTA	2314	OH2 TIP S	36	50.462	19.810	40.066	1.00 25.45	s
	ATOM	2315	OH2 TIP S	37	39.631	23.510	-0.239	1.00 30.88	s
	ATOM	2316	OH2 TIP S		44.734	42.655	10.346	1.00 30.84	s
	ATOM	2317	OH2 TIP S		54.653	3.902	1.503	1.00 30.04	S
5	ATOM	2318	OH2 TIP		45.693	21.923	39.754	1.00 27.14	
•	ATOM	2319	OH2 TIP S					•	S
			OH2 TIP S		47.820	16.413	7.805	1.00 25.73	S
	ATOM	2320			50.292	31.412	29.642	1.00 32.79	S
	MOTA	2321	OH2 TIP S		26.056	16.646	34.827	1.00 29.80	S
	MOTA	2322	OH2 TIP S	. –	31.714	10.996	31.855	1.00 29.15	S
10	MOTA	2323	OH2 TIP S	5 53	46.108	23.843	-4.299	1.00 24.21	s
	ATOM	2324	OH2 TIP S	5 54	37.645	11.206	34.448	1.00 28.56	S
	ATOM	-2325	OH2 TIP S	5 5 5	26.371	28.513	12.142	1.00 32.08	S
	ATOM	2326	OH2 TIP S	5 58	33.564	19.700	3.483	1.00 28.28	s
	ATOM	2327	OH2 TIP S	64	48.295	-0.632	14.280	1.00 32.13	S
15	ATOM	2328	OH2 TIP S		40.064	26.036	34.324	1.00 24.17	s
	ATOM	2329	OH2 TIP S		29.570	3.958	14.729	1.00 28.94	S
	ATOM	2330	OH2 TIP S		60.085	11.604	6.814	1.00 28.35	S
	ATOM	2331	OH2 TIP S		39.203	44.403			
							18.686	1.00 26.61	S
20	ATOM	2332	OH2 TIP S		47.312	12.366	27.366	1.00 28.51	S
20	ATOM	2333	OH2 TIP S		43.862	33.771	33.329	1.00 28.82	S
	ATOM	2334	OH2 TIP S		57.890	13.106	2.128	1.00 40.62	S
	MOTA	2335	OH2 TIP S		41.663	34.381	32.043	1.00 19.35	S
	ATOM	2336	OH2 TIP S		50.974	40.331	19.200	1.00 21.14	S
	MOTA	2337	OH2 TIP S	88	47.925	-0.832	-6.556	1.00 24.11	S
25	ATOM	2338	OH2 TIP S	90	27.231	28.336	33.481	1.00 27.64	S
	MOTA	2339	OH2 TIP S	91	43.651	-7.101	-7.995	1.00 24.33	S
	ATOM	2340	OH2 TIP S	92	49.325	4.387	19.370	1.00 28.02	S
	MOTA	2341	OH2 TIP S	93	46.231	11.549	33.898	1.00 29.40	s
	MOTA	2342	OH2 TIP S	94	63.889	24.831	1.168	1.00 26.53	s
30	ATOM	2343	OH2 TIP S	96	56.396	4.952	-6.749	1.00 28.00	s
	ATOM	2344	OH2 TIP S		35.510	27.986	11.558	1.00 29.24	S
	ATOM	2345	OH2 TIP S		49.942	24.366	30.265	1.00 31.61	s
	ATOM	2346	OH2 TIP S		56.121	7.113	-8.298	1.00 31.57	S
	ATOM	2347	OH2 TIP S		58.318	19.957	-8.378	1.00 26.95	S
35	ATOM	2348	OH2 TIP S		49.647	22.446	39.624	1.00 40.57	S
23	ATOM	2349	OH2 TIP S		45.359	7.052	13.052	1.00 26.27	S
	ATOM	2350	OH2 TIP S		37.150	32.340	32.346	1.00 26.27	S
									S
	ATOM	2351	OH2 TIP S		43.465	40.457	8.240	1.00 40.48	
40	ATOM	2352	OH2 TIP S		36.644		13.418	1.00 30.70	S
40	ATOM	2353	OH2 TIP S		41.912	-8.974	-8.264	1.00 26.08	s
	ATOM	2354	OH2 TIP S		62.424	15.800	-7.411	1.00 24.08	S
	ATOM	2355	OH2 TIP S		37.266	18.656	-9.097	1.00 28.99	S
	MOTA	2356	OH2 TIP S		43.129	26.845	14.606	1.00 25.19	S
	ATOM	2357	OH2 TIP S		36.339	32.639	29.802	1.00 29.25	S
45	MOTA	2358	OH2 TIP S	130	54.051	14.561	26.498	1.00 33.93	S
	ATOM	2359	OH2 TIP S	131	41.805	-4.242	5.492	1.00 33.72	·s
	ATOM	2360	OH2 TIP S	133	38.873	25.163	36.697	1.00 30.69	s
	MOTA	2361	OH2 TIP S		28.777	8.553	25.307	1.00 31.43	S
	ATOM	2362	OH2 TIP S		53.672	10.546	-12.803	1.00 33.45	S
50	ATOM	2363	OH2 TIP S		59.892	15.434	11.467	1.00 31.39	s
	ATOM	2364	OH2 TIP S		31.040	12.361	35.470	1.00 34.07	S
	ATOM	2365	OH2 TIP S		33.489	14.292	-0.598	1.00 40.68	s
	ATOM	2366	OH2 TIP S			8.748	11.662	1.00 29.23	S
	ATOM	2367	OH2 TIP S		46.297	-7.287	-9.196	1.00 29.23	S
55		2368	OH2 TIP S					1.00 42.20	S
55	ATOM				58.193	6.715	~4.685		
	ATOM	2369	OH2 TIP S		44.598	4.435	12.503	1.00 27.68	S
	ATOM	2370	OH2 TIP S		27.003	5.999	12.450	1.00 36.30	S
	ATOM	2371	OH2 TIP S		43.676	32.852	35.735	1.00 35.70	S
	MOTA	2372	OH2 TIP S	146	35.783	18.628	36.452	1.00 34.62	s

	ATOM	2373	OH2 TIP S	147	25.402	4.058	20.638	1.00 45.03	s
	MOTA	2374	OH2 TIP S	148	45.839	35.853	33.724	1.00 35.47	S
	ATOM	2375	OH2 TIP S	149	22.176	18.976	16.752	1.00 31.87	s
	MOTA .	2376	OH2 TIP S	150	43.986	33.179	10.162	1.00 37.70	S
5	MOTA	2377	OH2 TIP S	151	50.653	20.347	42.428	1.00 35.80	S
	ATOM	2378	OH2 TIP S	152	47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379	OH2 TIP S	153	44.693	5.273	-14.175	1.00 29.90	S
	ATOM	2380	OH2 TIP S	155	26.560	36.851	31.684	1.00 49.29	S
	ATOM	2381	OH2 TIP S	156	46.867		-12.951	1.00 29.21	S
10	ATOM	2382	OH2 TIP S	157	30.432	28.741	12.438	1.00 37.76	S
	ATOM	2383	OH2 TIP S		41.004	20.553	6.423	1.00 39.53	S
	ATOM	2384	OH2 TIP S		49.258	20.069	29.294	1.00 33.97	S
	ATOM	2385	OH2 TIP S		48.082	28.459	16.489	1.00 33.10	S
	ATOM	2386	OH2 TIP S		47.448	18.625	27.683	1.00 34.87	S
15	MOTA	2387	OH2 TIP S		19.687	20.632	23.411	1.00 35.01	S
	MOTA	2388	OH2 TIP S		32.402	-1.266	22.443	1.00 37.26	S
	ATOM	2389	OH2 TIP S		39.475	33.468	33.237	1.00 35.34	S
	ATOM	2390	OH2 TIP S		44.277	18.950	5.162	1.00 45.14	S
20	ATOM	2391	OH2 TIP S		34.797	30.523	10.736	1.00 47.55	S
20	ATOM	2392	OH2 TIP S		46.541	3.526	-14.949	1.00 26.54	S
	ATOM	2393	OH2 TIP S		36.333	16.371	1.539	1.00 38.68	S
	ATOM ATOM	2394	OH2 TIP S		46.761	38.936	27.403	1.00 34.66	S
	ATOM	2395 2396	OH2 TIP S OH2 TIP S		24.163	13.264	11.375	1.00 41.23	S
25	ATOM	2390		172	48.459 34.261	15.018	31.951	1.00 38.11	S
23	ATOM	2391		173	45.924	23.193 -0.026	40.004 13.224	1.00 48.96 1.00 39.55	S
	ATOM	2399	OH2 TIP S		41.384	37.389	32.543	1.00 39.55	s s
	ATOM	2400		177	49.394	35.312	27.150	1.00 40.74	S
	ATOM	2401		178	29.066	29.942	34.359	1.00 41.46	S
30	ATOM	2402		180	49.354	19.467	7.273	1.00 34.56	S
-	ATOM	2403	OH2 TIP S		25.298	17.029	31.863	1.00 47.74	s
	ATOM	2404	OH2 TIP S		37.071	25.027	4.669	1.00 43.87	S
	ATOM	2405	OH2 TIP S	183	22.581	7.487	18.691	1.00 41.75	S
	ATOM	2406	OH2 TIP S	184	32.269	7.011	-1.891	1.00 48.84	s
35	ATOM	2407	OH2 TIP S	185	48.234	0.494	6.833	1.00 48.16	S
•	ATOM	2408	OH2 TIP S	187	20.008	14.658	19.211	1.00 45.27	S
	MOTA	2409	OH2 TIP S	188	49.341	22.698	42.272	1.00 42.20	S
	ATOM	2410	OH2 TIP S	190	61.292	18.260	-8.097	1.00 45.21	S
	ATOM	2411	OH2 TIP S	191	28.152	10.606	2.819	1.00 40.38	S
40	ATOM	2412	OH2 TIP S	192	25.626	12.619	23.191	1.00 34.27	S
	ATOM	2413	OH2 TIP S	193	59.876	11.603	1.216	1.00 46.54	S
	ATOM	2414	OH2 TIP S	194	57.592	21.183	-10.646	1.00 45.82	S
	ATOM	2415		195	31.509	36.649	21.499	1.00 38.73	S
	ATOM	2416	OH2 TIP S		50.270	-1.543	-6.136	1.00 42.66	S
45	ATOM	2417	OH2 TIP S		24.467	8.729	13.088	1.00 42.78	S
	ATOM	2418	OH2 TIP S		38.098	8.699	25.759	1.00 32.80	S
	ATOM	2419	OH2 TIP S		57.831		-13.255	1.00 45.31	S
	ATOM	2420	OH2 TIP S		23.888	22.328	30.524	1.00 37.12	S
50	ATOM	2421	OH2 TIP S		47.691	26.068	37.666	1.00 37.92	S
50	ATOM	2422	OH2 TIP S		38.653	7.070	29.307	1.00 50.54	S
	ATOM	2423 2424	OH2 TIP S OH2 TIP S		44.424	27.583	2.092	1.00 53.50	s
	ATOM ATOM	2424	OH2 TIP S		22.258 19.843	2.296	17.948	1.00 47.38 1.00 30.36	s s
	ATOM	2425	OH2 TIP S		27.647	17.943 11.344	23.303	•	
55	ATOM	2420	OH2 TIP S		37.953	7.817	24.681 -9.284	1.00 31.32 1.00 45.97	s s
J.J	ATOM	2427	OH2 TIP S		33.845	34.040	$\frac{-9.264}{12.124}$	1.00 43.97	S
	ATOM	2429	OH2 TIP S		58.484	15.269	13.717	1.00 38.11	S
	ATOM	2430	OH2 TIP S		48.526	40.920	26.583	1.00 35.23	S
	ATOM	2431	OH2 TIP S		52.094	21.184	38.122	1.00 29.86	S.
			U		32.034		JU. 122		5

	MOTA	2432	OH2 TIP S 223	36.889	5.881	3.281	1.00 37.63	S
	ATOM	2433	OH2 TIP S 224	47.642		-10.684	1.00 34.89	S
	ATOM	2434	OH2 TIP S 226	47.284	2.916	19.133	1.00 34.10	S
	ATOM	2435	OH2 TIP S 227	42.468		-15.039	1.00 37.98	S
5	ATOM	2436	OH2 TIP S 228	19.169	22,832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S 231	57.592	12.689	14.880	1.00 50.22	S
	ATOM	2438	OH2 TIP S 232	27.102	9.176	5.655	1.00 30.22	
	ATOM	2439	OH2 TIP S 233	58.618		-11.925	1.00 40.37	s s
	ATOM	2440	OH2 TIP S 234	22.822	25.342	19.945	1.00 30.71	
10	ATOM	2441	OH2 TIP S 236	24.831	32.218		1.00 34.93	s s
- •	ATOM	2442	OH2 TIP S 237	20.045	10.774	16.992	1.00 37.69	
	ATOM	2443	OH2 TIP S 238		19.850	15.679	1.00 39.57	s s
	ATOM	2444	OH2 TIP S 239	19.490	20.949	26.114		
	ATOM	2445	OH2 TIP S 240	61.187	26.377	7.346	1.00 34.55	S
15	ATOM	2446	OH2 TIP S 241	33.680	38.342	19.389	1.00 39.66	S
12	ATOM	2447	OH2 TIP S 241	51.539	31.612	19.389	1.00 48.93	S
	ATOM	2448	OH2 TIP S 244	25.872	14.431	30.404		S
	ATOM	2449	OH2 TIP S 244	37.332	5.849	9.544	1.00 46.69 1.00 43.81	
	ATOM	2450	OH2 TIP S 250	39.087	-1.293	-9.655		S
20	ATOM	2451	OH2 TIP S 258	23.938	30.000	30.010	1.00 42.96	S
20	ATOM	2452	OH2 TIP S 259	24.949			1.00 38.89	s
	ATOM	2453	OH2 TIP S 259		29.749	32.578	1.00 40.17	S
	ATOM	2453	OH2 TIP S 266	32.111 21.404	17.986 12.876	1.918	1.00 48.36	s
	ATOM	2455	OH2 TIP S 269	35.425	36.767	25.603	1.00 57.17 1.00 30.70	S
25	ATOM	2456	OH2 TIP S 209	52.438	25.529	12.550 30.131		S
23	ATOM	2457		53.299	20.156	36.003	1.00 44.85 1.00 37.15	s s
	ATOM	2458	OH2 TIP S 272	50.914	6.919	23.723	1.00 37.13	S
	ATOM	2459	OH2 TIP S 274	31.578	30.795	11.014	1.00 43.29	S
	ATOM	2460	OH2 TIP S 275	26.341	7.243	22.447	1.00 30.13	S
30	ATOM	2461	OH2 TIP S 276	60.392	18.195	10.235	1.00 33.40	S
	ATOM	2462	OH2 TIP S 277	47.355		-10.821	1.00 37.31	s
	ATOM	2463	OH2 TIP S 279	41.304		-16.647	1.00 38.12	S
	ATOM	2464	OH2 TIP S 282	33.299	21.620	37.881	1.00 46.29	S
	ATOM	2465	OH2 TIP S 283	56.469	26.112	-8.575	1.00 43.71	S
35	ATOM	2466	OH2 TIP S 287		26.573	7.246	1.00 41.43	s
	ATOM	2467	OH2 TIP S 288	56.240			1.00 41.79	S
	ATOM	2468	OH2 TIP S 290	49.060	14.978	28.166	1.00 37.03	S
	ATOM	2469	OH2 TIP S 291	37.095	44.270	26.442	1.00 45.08	S
	ATOM	2470	OH2 TIP S 292	47.814		-13.299	1.00 48.60	S
40	ATOM	2471	OH2 TIP S 297	58.081	2.784	-7.841	1.00 41.89	s
	MOTA	2472	OH2 TIP S 298	36.447	45.321	18.644	1.00 54.91	S
	ATOM	2473	OH2 TIP.S 299	49.029	23.328	1.767	1.00 30.55	s
	ATOM	2474	OH2 TIP S 301	24.375	13.771	8.634	1.00 48.47	S
	ATOM	2475	OH2 TIP S 303	47.904	36.798	28.653	1.00 35.76	s
45	ATOM	2476	OH2 TIP S 305	51.156	40.821	27.172	1.00 43.59	S
	ATOM	2477	OH2 TIP S 306	32.943	28.917	35.227	1.00 42.60	S
	ATOM	2478	OH2 TIP S 307	58.462	28.373	6.251	1.00 46.15	S
	ATOM	2479	OH2 TIP S 308	41.964	30.940	36.712	1.00 48.26	S
	ATOM	2480	OH2 TIP S 313	51.176	-1.922	-3.336	1.00 50.61	S
50	MOTA	2481	OH2 TIP S1001	21.319	36.868	23.805	1.00 36.97	s
	ATOM	2482	OH2 TIP S1002	48.880	32.620	27.617	1.00 44.40	s
	MOTA	2483	OH2 TIP S1003	61.880	19.473	11.767	1.00 45.49	S
	ATOM	2484	OH2 TIP S1004	52.770	21.424	26.815	1.00 24.43	s
	ATOM	2485	OH2 TIP S1005	35.373	29.094	36.197	1.00 35.97	S
55	MOTA	2486	OH2 TIP S1006	40.815	-6.636	4.389	1.00 43.15	s
	MOTA	2487	OH2 TIP S1007	44.953	1.286	11.272	1.00 49.45	S
	ATOM	2488	OH2 TIP S1010	21.004	16.168	27.009	1.00 48.51	S
	ATOM	2489	OH2 TIP S1011	47.094	41.786	9.243	1.00 50.10	S
	MOTA	2490	OH2 TIP S1012	32.479	2.978	14.158	1.00 49.47	S

	ATOM	2491	O12 GLC G	1	48.557	11.372 -12.279	1.00 40.72	G
	ATOM	2492	C11 GLC G	1	48.836	12.133 -11.097	1.00 38.05	Ġ
	ATOM	2493	C13 GLC G	1	49.266	13.554 -11.476	1.00 38.09	G
	ATOM	2494	O14 GLC G	1	49.559	14.299 -10.292	1.00 33.99	G
5	ATOM	2495	C15 GLC G	1	48.150	14.257 -12.257	1.00 37.32	G
	ATOM	2496	O16 GLC G	1	48.574	15.582 -12.604	1.00 36.74	G
	ATOM	2497	O12 GLC G	2	40.114	-6.634 -6.562	1.00 33.52	G
	ATOM	2498	C11 GLC G	2	38.967	-6.592 -7.404	1.00 31.05	· G
	ATOM	2499	C13 GLC G	2	37.712	-6.417 -6.552	1.00 31.56	Ğ
10	ATOM	2500	O14 GLC G	2	36.554	-6.406 -7.389	1.00 30.70	G
	ATOM	2501	C15 GLC G	2	37.792	-5.109 -5.761	1.00 30.03	, G
	ATOM	2502	016 GLC G	2	36.609	-4.961 -4.975	1.00 29.66	G
	ATOM	2503	010 GLC G	3	44.030	8.243 -13.470	1.00 23.00	G
	ATOM	2504	C11 GLC G	3	43.950	9.648 -13.690	1.00 37.30	G
15	ATOM	2505	C13 GLC G	3	42.747	9.974 -14.579	1.00 30.47	G
13	ATOM	2506	O14 GLC G	3	41.551	9.526 -13.942	1.00 39.32	G
	ATOM	2507	C15 GLC G	3	42.878	9.280 -15.934	1.00 39.39	G
	ATOM	2508	016 GLC G	3	41.736	9.613 -16.731	1.00 41.43	, G
	ATOM	2509	O18 GLC G	5	40.556	1.005 2.289	1.00 45.78	G
20		2510	C11 GLC G	5	40.966	2.332 1.960	1.00 40.56	G
20	ATOM		C13 GLC G	5	40.187	3.327 2.814	1.00 40.36	G
	ATOM	2511		5				G
	ATOM	2512	O14 GLC G		38.791	3.169 2.572	1.00 40.71	
	ATOM	2513	C15 GLC G	5	40.619	4.751 2.464	1.00 40.04	G . G
۰.	ATOM	2514	O16 GLC G	5	39.885	5.681 3.256	1.00 36.89	•
25	MOTA	2515	O12 GLC G	6	36.951	22.702 40.046	1.00 63.04	G
	MOTA	2516	C11 GLC G	6	37.592	21.583 39.422	1.00 62.46	G
	ATOM	2517	C13 GLC G	6	38.104	21.978 38.030	1.00 61.14	G G
	MOTA	2518	O14 GLC G	6	39.034	23.054 38.168	1.00 61.72	
	ATOM	2519	C15 GLC G	6	36.948	22.429 37.126	1.00 60.51 1.00 58.61	G G
30	ATOM	2520	O16 GLC G	6	35.992	21.372 36.960		G
	MOTA	2521	O12 GLC G	7	37.316	0.281 14.299	1.00 73.45	G
	MOTA	2522	C11 GLC G	7	37.655	-0.758 15.222	1.00 72.78 1.00 72.98	. G
•	ATOM	2523	C13 GLC G	7	36.592	-1.856 15.157		G
25	ATOM	2524	O14 GLC G	7	35.320	-1.299 15.498	1.00 73.88 1.00 73.66	G
35	ATOM	2525	C15 GLC G	7	36.924	-2.989 16.134 -2.493 17.478	1.00 75.38	G
	ATOM	2526	O16 GLC G	7	36.972		1.00 75.38	G
	ATOM	2527	O12 GLC G	8	51.921	21.898 5.908 20.871 5.063	1.00 62.31	· G
	ATOM	2528	C11 GLC G	8	52.447	20.871 5.063 20.597 3.908	1.00 63.42	G
40	ATOM	2529	C13 GLC G	. 8	51.476		1.00 64.28	G
40	ATOM	2530	O14 GLC G	8	51.297	21.794 3.150 20.137 4.448	1.00 64.49	G
	ATOM	2531	C15 GLC G	8	50.121	19.886 3.357	1.00 64.49	G
	MOTA	2532		8	49.233		1.00 56.89	G
	MOTA	2533	O12 GLC G	10	36.044		1.00 56.89	G
45 .	ATOM	2534	C11 GLC G	10	35.164		1.00 56.11	_
45	MOTA	2535	C13 GLC G	10	33.849		1.00 56.44	. G G
	ATOM	2536	O14 GLC G	10	33.248	37.772 29.308	1.00 55.84	Ġ
	ATOM	2537	C15 GLC G		32.900	35.580 30.277 35.442 29.557	1.00 55.39	G
	ATOM	2538	O16 GLC G	10	31.674		1.00 55.39	N
50	ATOM	2539	O3G ATP N	1	46.280	25.658 5.170	1.00 51.49	N N
50	ATOM	2540	PG ATP N	1	46.464	25.053 3.691 23.911 3.763	1.00 52.22	N
	ATOM	2541	Olg ATP N	1	47.406			N
	MOTA	2542	O2G ATP N	1	46.794	26.182 2.784	1.00 52.07	
	ATOM	2543	O3B ATP N	1	44.976	24.513 3.344	1.00 51.01 1.00 50.20	N N
55	ATOM	2544	PB ATP N	1	44.560	22.969 3.605		
55	ATOM	2545	O1B ATP N	1	43.083	22.898 3.669	1.00 49.41 1.00 50.34	N
	MOTA	2546	O2B ATP N	1	45.345	22.474 4.766		N
	ATOM	2547	O3A ATP N	1	45.070	22.231 2.255	1.00 47.77	N
	ATOM	2548	PA ATP N	1	45.075	20.613 2.121	1.00 42.84	N
	MOTA	2549	O1A ATP N	1	45.547	20.291 0.754	1.00 43.81	N

	ATOM	2550		ATP			45.80	7	20.035	3.270	1.00	45.03	N	
	MOTA	2551		ATP			43.51	6	20.223	2.245	1.00	41.73	N	•
	MOTA	2552	C5*	ATP	N	1	42.52	8.	20.925	1.489	1.00	37.57	N	
	ATOM	2553	C4*	ATP	N	1	41.12	27	20.379	1.776	1.00	39.45	N	
5	ATOM	2554	04*	ATP	N	1	40.90	7	19.024	1.279	1.00	37.72	N	
	ATOM	2555	C3*	ATP	N	1	40.77	77	20.321			38.48	N	
	ATOM	2556		ATP			40.36		21.615			40.42	N	
	ATOM	2557	C2*				39.60		19.374	3.270		37.58	N	
	ATOM	2558		ATP			38.41		20.076			35.98	N	
10	MOTA	2559		ATP			39.93		18.346			35.55	N	
••	ATOM	2560	N9	ATP			40.62		17.156			31.76	N	
	ATOM	2561	C8	ATP			41.86		17.126			30.49		
	ATOM	2562	N7	ATP		1	42.14		15.877	3.667		29.75	N	
	ATOM	2563	C5	ATP		1	41.08		15.118	3.390			N	
15		2564				-						27.49	N	
13	ATOM		C4	ATP		1	40.12		15.925	2.810		30.02	N	
	ATOM	2565	ΝЗ.	ATP		1	38.93		15.389			27.11	N	
	ATOM	2566	C2	ATP		1	38.67		14.085	2.615		25.62	N	
	ATOM	2567	N1	ATP		1	39.59		13.283	3.175		21.76	N	
	MOTA	2568	C6	ATP		1	40.80		13.768	3.571		23.90	N	
20	ATOM	2569	N6	ATP		1.	41.69		12.964	4.127		21.94	N	
	MOTA	2570	S	SO4		1	58.68		8.493	~0.639		56.05	I	
	MOTA	2571	01	SO4		1	57.95	-	7.875	0.483		58.83	·I	
	ATOM	2572	02	SO4		1	57.88		9.607	-1.188		57.04	I	
	ATOM	2573	О3	SO4	Ι	1	58.90	6	7.478	-1.683	1.00	57.47	I	
25	MOTA	2574	04	SO4	I	1	59.97	6	9.008	-0.156	1.00	57.51	, I	
	MOTA	2575	S	SO4	I	2	39.33	9	4.855	7.057	1.00	84.24	I	
	ATOM	2576	01	SO4	1	2	39.39	0	6.175	7.711	1.00	85.02	I	
	MOTA	2577	02	SO4	Ι	2	40.10	1	4.897	5.797	1.00	84.75	I	
	ATOM	2578	03	SO4	I	2	37.93	6	4.506	6.766	1.00	84.94	I	
30	ATOM	2579	04	SO4	I	2	39.93	1	3.842	7.954	1.00	84.44	I	
	ATOM	2580	s	SO4	I	3	38.98	7	-2.256	3.310	1.00	58.58	I	
	MOTA	2581	01	SO4	I	3	37.73	4	-1.675	3.827	1.00	59.11	I	
	ATOM	2582	02	SO4	I	3	39.46	0	-1.454	2.172	1.00	59.91	I	
	ATOM	2583	03	SO4	I	3	38.74	3	-3.640	2.866	1.00	60.97	I	
35	ATOM	2584	04	SO4	I	3	40.01	4	-2.260	4.369	1.00	59.58	I	
-	ATOM	2585	S	SO4	I	4	34.39		5.289	30.981		64.34	I	
	ATOM	2586	01	SO4	I	4	33.62		6.528	30.742		60.43	I	
	ATOM	2587	02		I	4	34.33		4.427	29.782		60.11	I	
	ATOM	2588	03		I	4	33.81		4.572	32.133			. I	
40	ATOM	2589	04		ī	4	35.80		5.626	31.277		63.55	Ī	
٠٠.	ATOM	2590	S	SO4		5	55.07		-6.984	-3.711		75.40	ī	,
	ATOM	2591	01	SO4	Ī	5	54.65		-7.518	-2.399		74.66	ī	
	ATOM	2592	02		Ī	5	54.20		-5.845	-4.065		74.96	Ī	
	ATOM	2593	03	504		5	54.95		-8.034	-4.742		74.22	ī	
45	ATOM	2594	04	SO4		5	56.47		-6.532	-3.633		75.15	Ī	
73	ATOM	2595	02			100	57.36		24.998	13.149		66.76	P	
	ATOM	2596	03	PO4			59.39		26.166	13.761		66.89	. P	
	ATOM	2597	04	PO4			57.76		25.606	15.462		67.43	P	
50	ATOM	2598	01	PO4			57.26		27.325	13.818		65.91	P	
50	ATOM	2599	P	PO4	P		57.94		26.025	14.048		66.69	P	
	ATOM	2600	CB	GLU		80	50.41			-13.538		23.31	AC	
	ATOM	2601	CG	GLU		80	51.30			-14.362		24.09	AC	
	ATOM	2602	CD	GLU		80	52.180			-13.509		25.31	AC	
	ATOM	2603		GLU		80	52.84			-12.580		22.80	AC	
55	ATOM	2604		GLU		80	52.21			-13.774		28.07	AC	
	MOTA	2605	CB	SER		105	37.582		-1.281	-6.192		21.16	AC	
	ATOM	2606	OG	SER		105	37.12		-1.871	-4.988		20.42	AC	
	ATOM	2607	CB	ARG		116	59.520		22.977	-7.867		31.00	AC	
	ATOM	2608	CG	ARG		116	60.312	2	24.192	-8.323	0.50	32.50	AC	2

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MOTA
             2609 CD
                        ARG
                               116
                                         60.266
                                                  24.349
                                                          ~9.838
                                                                    0.50 34.11
                                                                                      AC2
                                                  25.499 -10.290
      ATOM
             2610
                        ARG
                    NE
                               116
                                         61.045
                                                                    0.50 36.67
                                                                                      AC2
      MOTA
             2611
                    CZ
                        ARG
                                                  26.766 -10.035
                               116
                                         60.729
                                                                    0.50 37.26
                                                                                      AC2
      MOTA
             2612
                    NH1 ARG
                               116
                                         59.642
                                                  27.053
                                                           -9.331
                                                                    0.50 38.99
                                                                                      AC2
      MOTA
             2613
                    NH2 ARG
                               116
                                         61.503
                                                  27.746 -10.479
                                                                    0.50 37.83
                                                                                      AC2
      MOTA
             2614
                    СВ
                        LEU
                               145
                                         49.693
                                                   8.642
                                                            6.631
                                                                    0.50 15.29
                                                                                      AC2
     ATOM
             2615
                    CG
                        LEU
                               145
                                         50.783
                                                   8.664
                                                            5.552
                                                                    0.50 14.29
                                                                                      AC2
     MOTA
             2616
                    CD1 LEU
                               145
                                         50.264
                                                   9.373
                                                            4.305
                                                                    0.50
                                                                          8.20
                                                                                      AC2
     MOTA
             2617
                    CD2 LEU
                               145
                                         52.030
                                                   9.361
                                                            6.087
                                                                    0.50 10.66
                                                                                      AC2
     MOTA
             2618
                    CB
                        ARG
                               183
                                       . 27.455
                                                  16.155
                                                           24.989
                                                                    0.50 19.21
                                                                                      AC2
     MOTA
             2619
                    CG
                        ARG
                               183
                                         28.077
                                                  15.397
                                                           26.147
                                                                    0.50 18.46
                                                                                      AC2
     ATOM
             2620
                    CD
                        ARG
                               183
                                         27.002
                                                  14.945
                                                           27.127
                                                                    0.50 19.72
                                                                                     AC2
     MOTA
             2621
                   NE
                        ARG
                               183
                                         26.016
                                                 14.086
                                                           26.478
                                                                    0.50 18.79
                                                                                     AC2
     MOTA
             2622
                    CZ
                        ARG
                               183
                                         24.703
                                                 14.279
                                                           26.539
                                                                    0.50 18.52
                                                                                     AC2
15
     ATOM
             2623
                   NH1 ARG
                               183
                                         24.213
                                                 15.305
                                                           27.221
                                                                    0.50 15.35
                                                                                     AC2
     ATOM
             2624
                   NH2 ARG
                               183
                                         23.881
                                                 13.445
                                                           25.915
                                                                    0.50 17.55
                                                                                     AC2
     MOTA
             2625
                   CB
                        SER
                               191
                                         38.479
                                                 10.847
                                                           23.036
                                                                   0.50 16.57
                                                                                     AC2
     MOTA
             2626
                   OG
                        SER
                               191
                                         37.418
                                                 10.765
                                                           23.973 0.50 18.62
                                                                                     AC2
     MOTA
             2627
                   CB
                        GLU
                               209
                                         38.645
                                                 24.079
                                                            8.551
                                                                   0.50 22.02
                                                                                     AC2
20
     ATOM
             2628
                        GLU
                   CG
                               209
                                         37.769
                                                 25.296
                                                            8.263
                                                                   0.50 23.40
                                                                                     AC2
     ATOM
             2629
                   CD
                        GLU
                               209
                                         37.513
                                                 26.175
                                                            9.483
                                                                   0.50 24.27
                                                                                     AC2
     MOTA
             2630
                   OE1
                       GLU
                               209
                                         37.076
                                                 27.328
                                                            9.288
                                                                   0.50 25.25
                                                                                     AC2
     MOTA
             2631
                       GLU
                               209
                   OE2
                                         37.737
                                                 25.727
                                                          10.629
                                                                   0.50 20.24
                                                                                     AC2
     MOTA
             2632
                   CB
                        GLN
                               247
                                         38.598
                                                 32.546
                                                          14.790
                                                                   0.50 18.71
                                                                                     AC2
25
     MOTA
             2633
                   CG
                        GLN
                               247
                                         38.077
                                                 33.665
                                                          13.900
                                                                   0.50 16.95
                                                                                     AC2
     MOTA
             2634
                   CD
                        GLN
                               247
                                         38.614
                                                 33.598
                                                          12.479
                                                                   0.50 19.13
                                                                                     AC2
     MOTA
                                         39.763
             2635
                   OE1
                       GLN
                               247
                                                 33.221
                                                          12.246
                                                                   0.50 17.24
                                                                                     AC2
     MOTA
             2636
                   NE2
                       GLN
                               247
                                         37.780
                                                 33.979
                                                          11.520
                                                                   0.50 19.88
                                                                                     AC2
     ATOM
             2637
                   CE
                        LYS
                               315
                                         34.978
                                                 25.150
                                                          36.369
                                                                   0.50 20.49
                                                                                     AC2
     ATOM
             2638
                   ΝZ
                        LYS
                               315
                                         34.183
                                                 24.074
                                                          37.023
                                                                   0.50 17.05
                                                                                     AC2
     MOTA
             2639
                   CB
                        GLN
                               352
                                        32.365
                                                  1.170
                                                          19.731
                                                                   0.50 31.10
                                                                                     AC2
     MOTA
             2640
                   CG
                        GLN
                               352
                                         33.833
                                                  0.778
                                                          19.683
                                                                   0.50 32.11
                                                                                     AC2
     ATOM
             2641
                   CD
                        GLN
                               352
                                         34.190
                                                  0.027
                                                          18.419
                                                                   0.50 33.04
                                                                                     AC2
     ATOM
             2642
                   OE1 GLN
                               352
                                        33.906
                                                  0.485
                                                          17.314
                                                                   0.50 34.87
                                                                                     AC2
35
     MOTA
             2643
                   NE2 GLN
                              352
                                        34.819
                                                 -1.133
                                                          18.575
                                                                   0.50 32.08
                                                                                     AC2
     END
```

Example 3: Co-ordinates for the PDK1 fragment without alternate side chains.

40

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 25.0 - 2.0 A
    REMARK starting r= 0.1972 free_r= 0.2220
    REMARK final
                    r= 0.1954 free r= 0.2224
    REMARK B rmsd for bonded mainchain atoms=
45
                                               1.501
                                                       target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.235
                                                      target= 2.0
    REMARK B rmsd for angle mainchain atoms= 2.347
                                                      target= 2.0
    REMARK B rmsd for angle sidechain atoms=
                                              3.302
    REMARK rweight= 0.0900 (with wa= 1.29263)
50
    REMARK target= mlf steps= 30
    REMARK sg= P3(2)21 a= 123.013 b= 123.013 c= 47.624 alpha= 90 beta= 90
    gamma= 120
    REMARK parameter file 1
                             : /ddl/david/projects/PDK1 new/CNS/prot.par
    REMARK parameter file 2
                             : /ddl/david/projects/PDK1_new/CNS/atp.par
55
    REMARK parameter file 3
                             : CNS_TOPPAR:water_rep.param
    REMARK parameter file 4
                             : CNS_TOPPAR:ion.param
```

```
REMARK parameter file 5 : /ddl/david/projects/PDKl_new/CNS/glycerol.par
     REMARK molecular structure file: ../generate/alternate.mtf
     REMARK input coordinates: ../minimize/minimize.pdb
     REMARK reflection file= ../../1/hkl/cns.hkl
     REMARK ncs= none
     REMARK B-correction resolution: 6.0 - 2.0
     REMARK initial B-factor correction applied to fobs :
     REMARK
               B11= -2.766 B22= -2.766 B33=
                                                 5.532
               B12= -0.375 B13=
     REMARK
                                  0.000 B23=
                                                 0.000
10
     REMARK B-factor correction applied to coordinate array B:
     REMARK bulk solvent: density level= 0.378441 e/A^3, B-factor= 52.6885 A^2
     REMARK reflections with |Fobs|/sigma F < 0.0 rejected .
     REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
     REMARK theoretical total number of refl. in resol. range:
                                                                      28210 ( 100.0
15
     육 )
     REMARK number of unobserved reflections (no entry or |F|=0):
                                                                        568 (
                                                                                 2.0
     ୫ )
     REMARK number of reflections rejected:
                                                                          0 (
                                                                                 0.0
20
     REMARK total number of reflections used:
                                                                      27642 (
                                                                                98.0
     REMARK number of reflections in working set:
                                                                      27063 (
                                                                               95.9
     REMARK number of reflections in test set:
                                                                        579 ( - 2.1
25
     용 )
                                47.624 90.00 90.00 120.00 P 32 2 1
     CRYST1 123.013 123.013
     REMARK FILENAME="bindividual.pdb"
     REMARK DATE:16-Apr-2002 18:31:12
                                              created by user: david
     REMARK VERSION:1.0
.30
     MOTA
                              71
               1 CB PRO A
                                      58.912 -7.251
                                                        8.216
                                                               1.00 67.78
                                                                                Α
     MOTA
               2
                  CG PRO A
                              71
                                      59.621
                                              -6.941
                                                        9.534
                                                               1.00 69.16
                                                                                Α
     MOTA
               3
                  С
                       PRO A
                              71
                                      59.493
                                              -6.506
                                                        5.894
                                                               1.00 67.06
     MOTA
               4
                       PRO A
                  0
                             71
                                      59.196
                                              -5.318
                                                        5.766
                                                               1.00 66.66
               5
     ATOM
                  N
                       PRO A
                              71
                                      60.984
                                              -6.073
                                                        7.833
                                                               1.00 67.86
                                                                                Α
35
                                                        9.207
     MOTA
               6
                  CD
                       PRO A
                              71
                                      60.554
                                              -5.762
                                                               1.00 68.24
                                                                                Α
     MOTA
               7 .
                  CA
                       PRO A
                              71
                                      60.040
                                              -7.035
                                                        7.217
                                                               1.00 67.75
                                                                                Α
     MOTA
               8
                  N
                       PRO A
                              72
                                      59.356
                                              -7.385
                                                        4.890
                                                               1.00 66.32
                                                                                Α
     MOTA
               9
                                      59.712
                  CD
                       PRO A
                              72
                                              -8.816
                                                        4.898
                                                               1.00 67.17
                                                                                Α
     ATOM
              10
                       PRO A
                                      58.840
                                              -6.986
                  CA
                              72
                                                        3.578
                                                               1.00 65.61
                                                                                Α
40
     ATOM
              11
                  CB
                       PRO A
                             .72
                                      58.672
                                              -8.321
                                                               1.00 66.47
                                                        2.858
                                                                                Α
     MOTA
              12
                                      59.796
                                              -9.133
                  CG
                       PRO A
                              72
                                                        3.419
                                                               1.00 67.57
                                                                                A
              13
     ATOM
                  С
                       PRO A
                              72
                                      57.527
                                              -6.208
                                                        3.673
                                                               1.00 63.94
     MOTA
              14
                  0
                       PRO A
                              72
                                      56.710
                                              -6.451
                                                        4.561
                                                               1.00 64.11
                                                                                Α
     MOTA
              15
                  N
                       ALA A
                              73
                                      57.341
                                              -5.268
                                                        2.753
                                                               1.00 61.57
                                                                                Α
45
     ATOM
              16
                 · CA
                      ALA A
                              73
                                      56.133
                                              -4.454
                                                        2.708
                                                               1.00 58.74
                                                                                Α
     ATOM
              17
                  CB
                      ALA A
                              73
                                      56.438
                                              -3.030
                                                        3.165
                                                               1.00 58.05
                                                                                Α
     MOTA
              18
                  С
                      ALA A
                              73
                                      55.626
                                              -4.448
                                                        1.271
                                                               1.00 56.78
                                                                                Α
     ATOM
              19
                  0
                                      56.347
                      ALA A
                              73
                                              -4.834
                                                        0.349
                                                               1.00 56.95
                                                                                Α
     ATOM
              20
                  N
                       PRO A
                              74
                                      54.372
                                              -4.024
                                                       1.057
                                                               1.00 54.15
                                                                                Α
50
     ATOM
              21
                  CD
                      PRO A
                              74
                                      53.335
                                              -3.610
                                                       2.018
                                                               1.00 53.31
                                                                                A
     MOTA
              22
                  CA
                      PRO A
                              74
                                      53.856
                                              -4.003
                                                      -0.314
                                                               1.00 52.54
                                                                                Α
     MOTA
              23
                  CB
                      PRO A
                              74
                                      52.474
                                              -3.375
                                                      -0.148
                                                              1.00 52.86
                                                                                Α
     ATOM
              24
                  CG
                      PRO A
                              74
                                      52.067
                                                              1.00 52.88
                                              -3.824
                                                       1.226
                                                                                Α
     MOTA
              25
                  С
                      PRO A
                              74
                                      54.772
                                              -3.167
                                                      -1.204
                                                               1.00 50.08
                                                                                Α
55
     MOTA
              26
                  0
                      PRO A
                              74
                                      55.559
                                              -2.361
                                                      -0.708
                                                               1.00 49.96
                                                                                Α
              27
     ATOM
                  N
                      ALA A
                              75
                                      54.680
                                              -3.366
                                                      -2.514
                                                               1.00 47.58
                                                                                Α
                             75
     ATOM
              28
                  CA
                      ALA A
                                      55.503
                                              -2.602
                                                      -3.446
                                                               1.00 44.69
                                                                                Α
     ATOM .
              29
                  CB
                             75
                                              -3.121
                                                               1.00 46.14
                      ALA A
                                      55.312
                                                      -4.870
                                                                               А
                             75
     MOTA
              30
                      ALA A
                                      55.100
                                              -1.134
                                                      -3.371
                                                              1.00 41.55
                                                                               Α
```

	•									
	ATOM	31	0	ALA A	75	53.947	7 -0.813	-3.086	1.00 41.01	A
	ATOM	32	N	LYS A	. 76	56.053	3 -0.245		1.00 38.31	. A
	ATOM	33	CA	LYS A	. 76	55.781			1.00 35.72	A
	ATOM	34	СВ	LYS A	. 76	57.053			1.00 37.70	A
5	ATOM	35	CG	LYS A	. 76	57.123			1.00 40.99	A
	ATOM	36	CD	LYS A		57.262			1.00 40.04	A
_	ATOM	37	CE	LYS A		57.511		-1.277	1.00 42.08	A
	ATOM	38	NZ	LYS A		57.681		0.202	1.00 42.99	A
	ATOM	39	C	LYS A		54.708	_	-4.638	1.00 32.65	A
10	ATOM	40	Ö	LYS A		54.814		-5.770	1.00 32.03	A
	ATOM	41	N	LYS A		53.668		-4.270	1.00 31.41	A
	ATOM	42	CA	LYS A		52.619		-5.232	1.00 25.72	A
	ATOM	43	СВ	LYS A		51.316		-4.509	1.00 25.72	A
	ATOM	44	CG	LYS A		50.796	-	-3.631	1.00 20.22	A
15	ATOM	45	CD	LYS A		49.487	_	-2.967	1.00 27.13	A A
٠.	ATOM	46	CE	LYS A		49.136		-1.870	1.00 20.30	
	ATOM	47	NZ	LYS A		48.998		-2.380	1.00 27.31	· A
	ATOM	48	C	LYS A	77	53.053		-6.137	1.00 27.17	A, A
	ATOM	49	0	LYS A	77	54.010		-5.829	1.00 24.67	A
20	ATOM	50	N	ARG A		52.351		-7.254	1.00 21.66	
	ATOM	51	CA	ARG A	78	52.662		-8.211	1.00 25.00	A A
	ATOM	52	CB	ARG A		53.574		-9.318	1.00 28.14	A
	ATOM	53	CG	ARG A	78	53.017		-10.050	1.00 28.37	A
	ATOM	54	CD	ARG A	78	54.092	•	-10.896	1.00 40.96	A
25	ATOM	55	NE	ARG A	78	53.560		-11.700	1.00 48.93	A
20	ATOM	56	CZ	ARG A	78	52.985		-11.203	1.00 52.58	A
	ATOM	57		ARG A	78	52.860		-9.889	1.00 52.50	A
	ATOM	58		ARG A	78	52.530		-12.022	1.00 54.09	A
	ATOM	59	C	ARG A	78	51.382		-8.803	1.00 23.76	A
30	ATOM	60	ŏ	ARG A	78	50.311		-8.706	1.00 24.25	A
50	ATOM	61	N	PRO A	79	51.475		-9.428	1.00 21.76	A
	ATOM	62	CD	PRO A	79	52.691		-9.668	1.00 20.82	A
	ATOM	63	CA	PRO A	79	50.301		-10.021	1.00 21.96	A
	ATOM	64	CB	PRO A	79	50.910		-10.816	1.00 22.27	A
35	ATOM	65	CG	PRO A	79	52.124		-10.014	1.00 22.12	A
	ATOM	66	C ·	PRO A	79	49.446		-10.903	1.00 22.86	A
	ATOM	67	0	PRO A	79	48.213		-10.842	1.00 20.52	A
	ATOM	68	N	GLU A	80	50.103		-11.714	1.00 21.87	A
	ATOM	69	CA	GLU A	80	49.403		-12.628	1.00 22.99	A
40	ATOM	70	СВ	GLU A	80	50.393		-13.571	1.00 25.24	A
	ATOM	71	CG	GLU A	80	51.230		-12.925	1.00 28.75	A
	MOTA	72	CD	GLU A	80	52.157		-13.913	1.00 31.99	А
	ATOM	73	OE1	GLU A	80	53.072	2.897	-14.433	1.00 34.34	А
-	ATOM	74	OE2	GLU A	80	51.969	1.015	-14.172	1.00 32.83	A
45	ATOM	75	С	GLU A	80	48.556	3.631	-11.912	1.00 22.09	A
	ATOM	76	0	GLU A	80	47.692		-12.530	1.00 22.37	A
	ATOM	77	N	ASP A	81	48.804		-10.622	1.00 19.97	Α
	ATOM	78	CA	ASP A	81	48.026	2.423	-9.874	1.00 19.93	A
	ATOM	79	CB	ASP A	81	48.736	2.029	-8.571	1.00 21.19	A
50	ATOM	80	CG	ASP A	·81	50.089	1.380	-8.807	1.00 22.46	A
	ATOM	81	OD1	ASP A	81	50.195	0.554	-9.731	1.00 24.22	A
	ATOM	82	OD2	ASP A	81	51.043	1.685	-8.058	1.00 23.33	A
	ATOM	83	С	ASP A	81	46.652	2.975	-9.518	1.00 20.85	А
	ATOM	84	Ó	ASP A	81	45.793		-9.015	1.00 19.96	A
55	ATOM	85	N	PHE A	82	46.445	4.258	-9.804	1.00 18.91	Α
	ATOM	86	CA	PHE A	82	45.200	4.934	-9.465	1.00 19.30	A
	ATOM	87	CB	PHE A	82	45.475	6.027	-8.427	1.00 18.43	A
	ATOM	88	CG	PHE A	82	46.134	5.531	-7.175	1.00 18.01	A
	ATOM	89	CD1	PHE A	82	45.371	5.136	-6.084	1.00 17.19	А

ATOM 91 CDZ PHE A 82 45.520 5.460 -7.086 1.00 18.99 A ATOM 92 CEZ PHE A 82 45.977 4.676 -4.918 1.00 17.12 A ATOM 93 CZ PHE A 82 45.977 4.676 -4.918 1.00 17.12 A ATOM 93 CZ PHE A 82 47.361 4.607 -4.838 1.00 18.00 A ATOM 95 CZ PHE A 82 47.361 4.607 -4.838 1.00 18.00 A ATOM 95 CZ PHE A 82 47.361 4.607 -4.838 1.00 18.00 B ATOM 95 CZ PHE A 82 45.066 5.936 -10.621 1.00 20.81 A ATOM 95 CZ PHE A 82 45.066 5.936 -10.621 1.00 20.81 A ATOM 95 CZ PHE A 82 45.066 5.936 -10.621 1.00 20.81 A ATOM 97 CA LYS A 83 42.321 6.478 -11.353 1.00 21.65 A ATOM 97 CA LYS A 83 42.321 6.478 -11.353 1.00 21.65 A ATOM 97 CA LYS A 83 42.321 6.478 -11.353 1.00 21.65 A ATOM 99 CG LYS A 83 41.096 5.625 -11.667 1.00 22.02 A ATOM 99 CG LYS A 83 41.096 5.625 -11.667 1.00 22.02 A ATOM 101 CZ PL LYS A 83 37.909 6.042 -12.550 1.00 28.93 A ATOM 101 CZ PL LYS A 83 37.909 6.042 -13.844 1.00 38.10 A ATOM 103 CZ LYS A 83 41.096 5.625 -11.657 1.00 22.02 A ATOM 104 CZ PL LYS A 83 37.909 6.042 -13.844 1.00 38.10 A ATOM 105 CZ PL LYS A 83 41.091 7.006 -13.043 1.00 43.33 A ATOM 105 CZ PL LYS A 83 41.091 7.006 -13.043 1.00 43.33 A ATOM 107 CZ PL LYS A 83 41.091 7.006 -13.043 1.00 43.33 A ATOM 107 CZ PL PHE A 84 42.513 8.848 -10.635 1.00 19.99 A ATOM 107 CZ PL PHE A 84 42.513 8.848 -10.635 1.00 18.63 A ATOM 107 CZ PL PHE A 84 42.513 8.848 -10.635 1.00 18.63 A ATOM 107 CZ PHE A 84 44.579 1.0741 -9.587 1.00 17.66 A ATOM 110 CZ PHE A 84 44.579 1.0741 -9.587 1.00 17.66 A ATOM 110 CZ PHE A 84 44.549 11.034 -9.560 1.00 18.16 A ATOM 110 CZ PHE A 84 44.549 11.034 -9.560 1.00 18.16 A ATOM 111 CZ PHE A 84 44.6571 10.741 -9.587 1.00 17.66 A ATOM 112 CZ PHE A 84 44.6571 10.741 -9.587 1.00 17.03 A A ATOM 113 CZ PHE A 84 44.849 11.183 -8.299 1.00 18.66 A ATOM 113 CZ PHE A 84 44.849 11.183 -8.299 1.00 18.66 A ATOM 113 CZ PHE A 84 44.849 11.183 -9.586 1.00 18.16 A ATOM 113 CZ PHE A 84 44.6576 -9.556 -9.589 1.00 18.09 A ATOM 113 CZ PHE A 84 44.6571 10.741 -9.587 1.00 17.09 A ATOM 113 CZ PHE A 84 44.591 10.104 -9.587 1.00 17.09 A ATOM 113 CZ PHE A 84 44.591 10.00 -9.766 1.00 12.72									•			
ATOM 93 CZ PHE A 82 48.137 5.000 -5.925 1.00 19.64 A A A A A C PHE A 82 44.476 5.596 -10.621 1.00 20.81 A A A A A C PHE A 82 44.476 5.596 -10.621 1.00 20.81 A A A A C PHE A 82 44.476 5.596 -10.621 1.00 20.81 A A A A C PHE A 82 44.476 5.596 -10.621 1.00 20.81 A A A A C PHE A 82 44.476 5.596 -10.621 1.00 20.34 A A A A C PHE A 82 45.666 5.933 -11.699 1.00 20.34 A A A C PHE A 82 45.666 5.933 -11.699 1.00 20.34 A A A P P P P P P P P P P P P P P P P		ATOM	90	CD2	PHE A	82	•	47.520	5.460	-7.086	1.00 18.99	A
ATOM 94 C PHE A 82 47.361 4.607 -4.838 1.00 18.00 A A A A A A A A A A A A A A A A A A		MOTA	91	CE1	PHE A	82	•	45.977	4.676	-4.918	1.00 17.12	· A
S		MOTA	92	CE2	PHE A	82		48.137	5.000	-5.925	1.00 19.64	A
ATOM 95 O PHE A 82 45.066 5.933 -11.649 1.00 20.34 A A ATOM 95 N LYS A 83 43.182 5.752 -10.411 1.00 19.80 A A A ATOM 97 CA LYS A 83 43.182 5.752 -10.411 1.00 19.80 A A A ATOM 99 CB LYS A 83 41.096 5.625 -11.687 1.00 22.02 A A ATOM 99 CG LYS A 83 41.096 5.625 -12.550 1.00 22.02 A A ATOM 101 CC LYS A 83 38.974 5.355 -12.981 1.00 34.20 A A ATOM 101 CC LYS A 83 38.974 5.355 -12.981 1.00 34.20 A A A A A A A A A A A A A A A A A A A		MOTA	93	CZ	PHE A	82		47.361	4.607	-4.838	1.00 18.00	A
ATOM 95 N LYS A 83 42.182 5.792 -10.411 1.00 19.80 A A ATOM 97 CA LYS A 83 42.321 6.478 -11.353 1.00 21.65 A A ATOM 98 CB LYS A 83 40.062 6.326 -12.550 1.00 22.02 A A ATOM 100 CD LYS A 83 40.062 6.326 -12.550 1.00 28.93 A A A A A A A A A A A A A A A A A A A	5	MOTA	94	С	PHE A	82		44.476	5.596	-10.621	1.00 20.81	A
ATOM 98 CB LYS A 83 42.321 6.478 -11.353 1.00 21.65 A ATOM 99 CG LYS A 83 40.062 6.326 -12.550 1.00 22.02 A ATOM 100 CD LYS A 83 38.974 5.355 -12.981 1.00 34.20 A ATOM 101 CE LYS A 83 37.979 6.042 -13.824 1.00 34.20 A ATOM 102 NZ LYS A 83 37.179 7.086 -13.043 1.00 43.33 A ATOM 103 C LYS A 83 37.179 7.086 -13.043 1.00 43.33 A ATOM 103 C LYS A 83 41.913 7.702 -10.541 1.00 20.74 A ATOM 105 N PHE A 84 42.513 8.488 -10.835 1.00 20.98 A ATOM 106 CA PHE A 84 42.188 10.049 -10.083 1.00 19.99 A ATOM 107 CB PHE A 84 42.188 10.049 -10.083 1.00 18.63 A ATOM 108 CG PHE A 84 44.571 10.741 -9.587 1.00 17.68 A ATOM 109 CD1 PHE A 84 44.571 10.741 -9.587 1.00 17.68 A ATOM 110 CD2 PHE A 84 44.843 11.183 -8.299 1.00 18.65 A ATOM 110 CD2 PHE A 84 46.676 9.555 -9.589 1.00 19.66 A ATOM 111 CC2 PHE A 84 46.676 9.555 -9.589 1.00 19.66 A ATOM 112 CE2 PHE A 84 46.676 9.555 -9.589 1.00 19.69 A ATOM 113 CZ PHE A 84 46.021 10.816 -7.653 1.00 18.89 A ATOM 114 C PHE A 84 40.931 10.816 -7.653 1.00 18.89 A ATOM 115 O PHE A 84 40.391 10.489 -11.601 1.00 20.72 A ATOM 116 N GLY A 85 38.872 11.810 -9.716 1.00 17.33 A ATOM 116 N GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 117 CA GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 118 C GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 119 C GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 120 N LYS A 86 37.573 13.604 -9.855 1.00 18.55 A ATOM 120 N LYS A 86 36.133 15.302 -7.812 1.00 18.05 A ATOM 121 C CE2 LYS A 86 36.33.994 14.606 -6.481 1.00 17.73 A ATOM 122 CB LYS A 86 36.33.994 14.607 -8.855 1.00 18.75 A ATOM 124 CD LYS A 86 36.33.994 14.607 -8.855 1.00 18.75 A ATOM 125 CE LYS A 86 36.33.994 14.607 -8.855 1.00 18.55 A ATOM 122 CB LYS A 86 36.35.994 14.607 -8.855 1.00 18.57 A ATOM 123 CG LYS A 86 36.35.994 17.529 -9.858 1.00 18.57 A ATOM 124 CD LYS A 86 36.35.994 17.529 -9.855 1.00 18.57 A ATOM 125 CE LYS A 86 36.35.994 17.629 -9.855 1.00 18.57 A ATOM 130 CA LLE A 87 39.577 17.554 -6.256 1.00 18.57 A ATOM 131 CG LYS A 86 36.35.999 19.86 -5.628 1.00 18.57 A ATOM 133 CG LIE A 87 40.599 19.786 -5.628 1.0		MOTA	95	0	PHE A	82		45.066	5.933	-11.649	1.00 20.34	A
ATOM		ATOM	96	N	LYS A	83		43.182	5.792	-10.411	1.00 19.80	A
10		ATOM	97	CA	LYS A	83		42.321	6.478	-11.353	1.00 21.65	A
ATOM 100 CD LYS A 83 38.974 5.355 -12.981 1.00 34.20 A ATOM 101 CE LYS A 83 37.909 6.042 -13.824 1.00 38.10 A A ATOM 102 NZ LYS A 83 37.179 7.086 -13.043 1.00 38.10 A A ATOM 103 C LYS A 83 41.913 7.702 -10.541 1.00 20.74 A ATOM 104 O LYS A 83 41.913 7.702 -10.541 1.00 20.74 A ATOM 106 CA PHE A 84 42.513 8.848 -10.835 1.00 19.99 A ATOM 106 CA PHE A 84 42.513 8.848 -10.835 1.00 19.99 A ATOM 107 CB PHE A 84 42.518 10.049 -10.0083 1.00 18.63 A ATOM 108 CG PHE A 84 44.571 10.741 -9.587 1.00 17.58 A ATOM 108 CG PHE A 84 44.571 10.741 -9.587 1.00 17.58 A ATOM 101 CD2 PHE A 84 44.571 10.741 -9.587 1.00 18.95 A ATOM 110 CD2 PHE A 84 44.571 10.741 -9.587 1.00 18.09 A ATOM 111 CE1 PHE A 84 46.021 10.816 -7.653 1.00 18.09 A ATOM 111 CE1 PHE A 84 46.021 10.816 -7.653 1.00 18.09 A ATOM 112 CE2 PHE A 84 46.021 10.816 -7.653 1.00 18.09 A ATOM 113 CZ PHE A 84 46.021 10.816 -7.653 1.00 18.09 A ATOM 113 CZ PHE A 84 46.021 10.816 -7.653 1.00 18.09 A ATOM 113 CZ PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 120 N LYS A 85 38.872 11.830 -9.484 1.00 16.80 A ATOM 120 N LYS A 86 37.571 15.064 -8.278 1.00 18.75 A ATOM 120 C LYS A 86 37.571 15.064 -8.278 1.00 18.75 A ATOM 120 C LYS A 86 37.571 15.064 -8.278 1.00 18.75 A ATOM 122 CB LYS A 86 37.571 15.064 -8.278 1.00 18.55 A ATOM 122 CB LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 122 CB LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 123 CG LYS A 86 33.994 14.239 -4.793 1.00 31.924 A ATOM 125 CB LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 126 CD LYS A 86 33.994 14.239 -4.793 1.00 31.926 A ATOM 127 C LYS A 86 33.994 14.239 -4.793 1.00 18.56 A ATOM 128 CD LYS A 86 33.994 14.239 -4.793 1.00 18.57 A ATOM 128 CD LYS A 86 33.994 14.239 -4.793 1.00 18.56 A ATOM		ATOM	98	CB	LYS A	83		41.096	5.625	-11.687	1.00 22.02	A
ATOM 101 CE LYS A 83 37.599 6.042 -13.824 1.00 38.10 A ATOM 103 C LYS A 83 37.179 7.086 -13.043 1.00 43.33 A ATOM 103 C LYS A 83 41.913 7.702 -10.541 1.00 20.74 A ATOM 105 N PHE A 84 42.513 8.848 -10.835 1.00 19.99 A ATOM 106 CA PHE A 84 42.518 8.848 -10.835 1.00 19.99 A ATOM 107 CB PHE A 84 42.513 8.848 -10.258 1.00 19.99 A ATOM 108 CG PHE A 84 42.513 10.741 -9.587 1.00 18.95 A ATOM 109 CD1 PHE A 84 44.571 10.741 -9.587 1.00 18.95 A ATOM 110 CD2 PHE A 84 44.571 10.741 -9.587 1.00 18.95 A ATOM 110 CD2 PHE A 84 44.843 11.83 -8.299 1.00 19.66 A ATOM 111 CE1 PHE A 84 46.676 9.556 -9.589 1.00 19.66 A ATOM 112 CE2 PHE A 84 46.021 10.816 -7.653 1.00 19.99 A ATOM 113 CZ PHE A 84 46.021 10.816 -7.653 1.00 19.66 A ATOM 114 C PHE A 84 46.936 10.002 -8.301 1.00 19.66 A ATOM 115 O PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 116 N GLY A 85 38.872 11.810 -9.716 1.00 19.69 A ATOM 117 CA GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 118 C GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 120 N LYS A 86 37.571 15.064 -9.560 1.00 17.73 A ATOM 121 CA LYS A 86 37.571 15.064 -9.6276 1.00 18.45 A ATOM 122 CB LYS A 86 37.571 15.064 -9.6276 1.00 18.45 A ATOM 124 CD LYS A 86 37.571 15.064 -9.6276 1.00 18.56 A ATOM 125 CE LYS A 86 37.571 15.064 -9.650 1.00 18.56 A ATOM 126 NZ LYS A 86 37.571 15.064 -9.6276 1.00 18.56 A ATOM 127 C LYS A 86 37.571 15.064 -9.6278 1.00 18.56 A ATOM 128 C LYS A 86 37.571 15.064 -9.6278 1.00 18.56 A ATOM 126 NZ LYS A 86 37.571 15.064 -9.6278 1.00 18.56 A ATOM 127 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 127 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 126 NZ LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 127 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 C LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 NZ LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 NZ LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 128 NZ LYS A 86 37.571 15.064 -9.650 1.00 18.55 A ATOM 129 NZ LYS	10	ATOM	99	CG	LYS A	83		40.062	6.326	-12.550	1.00 28.93	A
ATOM 102 NZ LYS A 83 41.913 7.086 -13.043 1.00 43.33 A ATOM 104 O LYS A 83 41.913 7.702 -10.541 1.00 20.74 A ATOM 105 N PHE A 84 42.513 8.848 -10.835 1.00 19.99 A ATOM 106 CA PHE A 84 42.188 10.049 -10.835 1.00 18.63 A ATOM 107 CB PHE A 84 42.188 10.049 -10.835 1.00 18.63 A ATOM 108 CG PHE A 84 42.188 10.049 -10.835 1.00 18.65 A ATOM 109 CD1 PHE A 84 44.571 10.741 -9.587 1.00 18.66 A ATOM 110 CD2 PHE A 84 44.571 10.741 -9.587 1.00 18.66 A ATOM 111 CD2 PHE A 84 44.843 11.183 -8.299 1.00 18.16 A ATOM 111 CD2 PHE A 84 46.676 9.556 -9.559 1.00 18.09 A ATOM 111 CZ PHE A 84 46.676 9.556 -9.559 1.00 18.09 A ATOM 113 CZ PHE A 84 46.936 10.002 -8.301 1.00 18.99 A ATOM 113 CZ PHE A 84 40.931 10.617 -10.460 1.00 19.69 A ATOM 115 O PHE A 84 40.391 10.489 -11.601 1.00 20.72 A ATOM 116 N GLY A 85 38.819 11.233 -9.484 10.017 -3.33 A ATOM 117 CA GLY A 85 38.819 13.280 -9.346 1.00 16.80 A ATOM 118 C GLY A 85 38.819 13.280 -9.346 1.00 16.80 A ATOM 119 O GLY A 85 39.740 14.043 -9.556 1.00 18.75 A ATOM 120 CG LY A 85 39.740 14.043 -9.650 1.00 18.75 A ATOM 121 CA LYS A 86 37.753 13.673 -8.659 1.00 18.56 A ATOM 122 CG LYS A 86 36.133 15.302 -7.812 1.00 18.75 A ATOM 123 CG LYS A 86 36.5793 14.600 -6.861 1.00 21.55 A ATOM 124 CD LYS A 86 38.5793 14.600 -6.861 1.00 21.55 A ATOM 125 C LYS A 86 38.5793 15.004 -9.236 1.00 18.77 A ATOM 126 CG LYS A 86 38.523 15.571 -7.222 1.00 19.03 1.92 A ATOM 127 C LYS A 86 39.545 14.807 -6.385 1.00 18.77 A ATOM 128 C LYS A 86 39.545 14.807 -6.385 1.00 18.77 A ATOM 128 C LYS A 86 39.593 14.660 -6.661 1.00 21.55 A ATOM 129 N LLE A 87 39.994 18.952 -6.772 1.00 19.07 A ATOM 130 CA LLE A 87 39.994 18.952 -6.772 1.00 19.07 A ATOM 131 CB LLE A 87 39.577 17.554 -6.256 1.00 18.77 A ATOM 130 CA LLE A 87 39.577 17.554 -6.256 1.00 19.15 A ATOM 130 CA LLE A 87 39.577 17.554 -6.256 1.00 19.00 18.57 A ATOM 130 CA LLE A 87 39.994 18.952 -6.772 1.00 19.00 19.00 A ATOM 131 CB LLE A 87 39.994 18.952 -6.772 1.00 19.00 19.00 A ATOM 130 CA LLE A 87 39.577 17.554 -6.256 1.00 19.00 19.00 A ATOM 130 CA LLE A 87 39.577 17.554 -6		MOTA	100	CD	LYS A	83		38.974	5.355	-12.981	1.00 34.20	A
ATOM		ATOM	101	CE	LYS A	83		37.909	6.042	-13.824	1.00 38.10	A
15		MOTA	102	NZ	LYS A	83		37.179	7.086	-13.043	1.00 43.33	Α
ATOM		MOTA	103	С	LYS A	83		41.913	7.702	-10.541	1.00 20.74	A
ATOM	15	ATOM	104	0	LYS A	83		41.084	7.606	-9.635	1.00 20.98	A
ATOM		ATOM	105	N	PHE A	84		42.513	8.848	-10.835	1.00 19.99	A
ATOM		ATOM	106	CA	PHE A	84		42.188	10.049	-10.083	1.00 18.63	A
ATOM		ATOM	107	СВ	PHE A	84		43.279	11.103	-10.258	1.00 18.95	A
ATOM			108	CG	PHE A	84		44.571	10.741	-9.587	1.00 17.68	A
ATOM	20		109	CD1	PHE A	84		45.498	9.926	-10.224	1.00 18.16	A
ATOM 111 CEL PHE A 84 46.676 9.556 -9.589 1.00 18.09 A ATOM 112 CE2 PHE A 84 46.021 10.816 -7.653 1.00 18.89 A ATOM 113 CZ PHE A 84 46.036 10.002 -8.301 1.00 17.33 A 25 ATOM 114 C PHE A 84 40.834 10.617 -10.460 1.00 19.69 A ATOM 115 O PHE A 84 40.391 10.489 -11.601 1.00 20.72 A ATOM 116 N GLY A 85 40.178 11.233 -9.484 1.00 16.80 A ATOM 117 CA GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 118 C GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 119 O GLY A 85 39.740 14.043 -9.650 1.00 18.75 A ATOM 120 N LYS A 86 37.753 13.673 -8.659 1.00 18.45 A ATOM 121 CA LYS A 86 37.753 13.673 -8.659 1.00 18.26 A ATOM 122 CB LYS A 86 37.753 13.673 -8.659 1.00 18.26 A ATOM 123 CG LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 124 CD LYS A 86 33.994 14.239 -4.793 1.00 31.92 A ATOM 125 CE LYS A 86 33.994 14.239 -4.793 1.00 31.92 A ATOM 126 NZ LYS A 86 38.523 15.571 -7.022 1.00 18.57 A ATOM 127 C LYS A 86 38.523 15.571 -7.022 1.00 18.57 A ATOM 128 O LYS A 86 38.523 15.571 -7.227 1.00 18.57 A ATOM 127 C LYS A 86 38.523 15.571 -7.227 1.00 18.57 A ATOM 128 O LYS A 86 38.523 15.571 -7.227 1.00 18.57 A ATOM 127 C LYS A 86 38.523 15.571 -7.227 1.00 18.57 A ATOM 128 O LYS A 86 38.523 15.571 -7.227 1.00 18.57 A ATOM 129 N ILE A 87 39.577 17.554 -6.556 1.00 18.57 A ATOM 130 CA ILE A 87 39.994 18.952 -6.772 1.00 18.26 A ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 133 CG1 ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 134 CD1 ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 135 C ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 137 N LEU A 88 39.995 19.709 -2.237 1.00 19.97 A ATOM 138 CA LEU A 88 38.800 16.151 -1.700 1.00 19.97 A ATOM 137 N LEU A 88 39.997 19.174 -2.179 1.00 19.01 A ATOM 140 CG LEU A 88 38.800 16.551 -1.901 1.00 20.11 A ATOM 141 CD1 ILE A 88 39.999 19.146 -1.1507 1.00 24.09 A ATOM 144 CD2 LEU A 88 39.999 19.146 -1.1507 1.00 24.09 A ATOM 144 CD2 LEU A 88 39.999 19.146 -1.1507 1.00 24.09 A ATOM 144 CD2 LEU A 88 39.999 19.146 -1.507 1.00 24.09 A ATOM 144 C C GLY A 89 39.999 19.146 -1.507 1.00 24.07 A						84					1.00 19.66	A
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ATOM			112	CE2	PHE A	84		46.021	10.816	-7.653	1.00 18.89	А
25				CZ	PHE A	84			10.002	-8.301	1.00 17.33	А
ATOM 115 O PHE A 84 40.391 10.489 -11.601 1.00 20.72 A ATOM 116 N GLY A 85 40.178 11.233 -9.484 1.00 16.80 A ATOM 117 CA GLY A 85 38.872 11.810 -9.716 1.00 17.73 A A ATOM 118 C GLY A 85 38.819 13.280 -9.346 1.00 18.75 A ATOM 120 N LYS A 86 37.753 13.673 -8.659 1.00 18.45 A ATOM 121 CA LYS A 86 37.753 13.673 -8.659 1.00 18.26 A ATOM 121 CA LYS A 86 37.571 15.064 -8.278 1.00 19.00 A ATOM 122 CB LYS A 86 36.133 15.302 -7.812 1.00 19.00 A ATOM 123 CG LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 124 CD LYS A 86 33.994 14.239 -4.793 1.00 31.92 A ATOM 125 CE LYS A 86 33.994 14.239 -4.793 1.00 31.92 A ATOM 127 C LYS A 86 33.594 14.457 -4.412 1.00 35.36 A ATOM 127 C LYS A 86 38.523 15.571 -7.202 1.00 18.57 A ATOM 128 O LYS A 86 38.523 15.571 -7.202 1.00 18.57 A ATOM 129 N LLE A 87 38.537 16.881 -7.227 1.00 17.88 A ATOM 130 CA LLE A 87 39.994 18.952 -6.772 1.00 17.88 A ATOM 131 CB LLE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 133 CG1 LLE A 87 40.593 19.786 -5.628 1.00 19.60 A ATOM 133 CG1 LLE A 87 40.593 19.786 -5.628 1.00 19.60 A ATOM 133 CG1 LLE A 87 40.593 19.786 -5.628 1.00 19.60 A ATOM 133 CG1 LLE A 87 40.593 19.786 -5.628 1.00 19.60 A ATOM 133 CG1 LLE A 87 40.593 19.786 -5.628 1.00 19.60 A ATOM 135 CG LLE A 87 40.593 19.786 -5.628 1.00 19.67 A ATOM 136 CO LLE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.67 A ATOM 136 CO LLE A 87 39.994 18.952 -6.772 1.00 19.67 A ATOM 137 N LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 137 N LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 137 N LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 137 N LEU A 88 38.509 17.324 -2.611 1.00 20.68 A ATOM 137 N LEU A 88 38.509 17.324 -2.611 1.00 21.41 A ATOM 140 CG LEU A 88 38.509 17.324 -2.611 1.00 20.68 A ATOM 143 C LEU A 88 38.509 17.324 -2.611 1.00 20.68 A ATOM 143 C LEU A 88 38.509 17.324 -2.611 1.00 20.68 A ATOM 143 C LEU A 88 38.509 17.324 -2.611 1.00 21.41 A ATOM 140 CG LEU A 88 38.509 17.324 -2.611 1.00 22.11 A ATOM 141 CD1 LEU A 88 38.509 17.324 -2.611 1.00 22.11 A ATOM 142 CD2 LEU A	25											A
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ATOM 118 C GLY A 85 38.872 11.810 -9.716 1.00 17.73 A ATOM 118 C GLY A 85 38.819 13.280 -9.346 1.00 18.75 A ATOM 119 O GLY A 85 39.740 14.043 -9.650 1.00 18.45 A ATOM 120 N LYS A 86 37.753 13.673 -8.659 1.00 16.00 A ATOM 121 CA LYS A 86 37.571 15.064 -8.278 1.00 18.26 A ATOM 122 CB LYS A 86 36.133 15.302 -7.812 1.00 19.00 A ATOM 123 CG LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 124 CD LYS A 86 35.793 14.660 -6.481 1.00 21.55 A ATOM 125 CE LYS A 86 34.368 14.981 -6.066 1.00 26.48 A ATOM 125 CE LYS A 86 33.994 14.239 -4.793 1.00 31.92 A ATOM 127 C LYS A 86 38.523 15.571 -7.202 1.00 18.57 A ATOM 127 C LYS A 86 38.523 15.571 -7.202 1.00 18.57 A ATOM 128 O LYS A 86 39.045 14.807 -6.385 1.00 16.77 A ATOM 128 O LYS A 86 39.045 14.807 -6.385 1.00 16.77 A ATOM 130 CA LEE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 131 CB LEE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 133 CGI LLE A 87 39.994 18.952 -6.772 1.00 17.88 A ATOM 133 CGI LLE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CGI LLE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CGI LLE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 135 C LLE A 87 38.737 17.554 -6.256 1.00 18.73 A ATOM 136 O LLE A 87 38.731 17.709 -4.997 1.00 19.60 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.67 A ATOM 138 CA LEU A 88 39.240 17.229 -3.867 1.00 19.67 A ATOM 136 O LLE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 137 N LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 139 CB LEU A 88 38.508 17.324 -2.611 1.00 20.41 A ATOM 140 CG LEU A 88 38.508 17.324 -2.611 1.00 20.41 A ATOM 141 CDL LEU A 88 38.509 14.759 -2.237 1.00 19.97 A ATOM 142 CDL LEU A 88 38.509 14.759 -2.237 1.00 19.97 A ATOM 142 CDL LEU A 88 38.509 14.759 -2.237 1.00 19.91 A ATOM 143 C LEU A 88 38.509 14.759 -2.237 1.00 19.91 A ATOM 141 CDL LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 142 CDL LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 143 C LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 143 C LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 144 C CDL LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 144 C CDL						85		40.178	11.233	-9.484		· · A
ATOM												А
ATOM								38.819	13.280	-9.346	1.00 18.75	A
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ATOM							*				1.00 21.55	А
ATOM 125 CE	35								14.981	-6.066	1.00 26.48	A
ATOM 126 NZ LYS A 86 32.568 14.457 -4.412 1.00 35.36 A ATOM 127 C LYS A 86 38.523 15.571 -7.202 1.00 18.57 A ATOM 128 O LYS A 86 39.045 14.807 -6.385 1.00 16.77 A ATOM 129 N ILE A 87 38.737 16.881 -7.227 1.00 17.88 A ATOM 130 CA ILE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 19.73 A ATOM 133 CG1 ILE A 87 40.593 19.786 -7.945 1.00 21.16 A ATOM 135 C ILE A 87 40.968 18.786 -7.945 1.00 21.16 A ATOM 135 C ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 136 O ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 20.41 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 139 CB LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 140 CG LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 140 CG LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 141 CD1 LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 140 CG LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 140 CG LEU A 88 38.508 17.324 -2.611 1.00 20.68 A ATOM 141 CD1 LEU A 88 38.509 14.759 -2.237 1.00 19.97 A ATOM 140 CG LEU A 88 38.509 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 25.47					-7							Α
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ATOM 128 O LYS A 86 39.045 14.807 -6.385 1.00 16.77 A 40 ATOM 129 N ILE A 87 38.737 16.881 -7.227 1.00 17.88 A ATOM 130 CA ILE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A 45 ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.27 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 37.029 14.622 -2.359 1.00 23.11 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.27 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.27 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.27 A ATOM 147 C GLY A 89 40.367 20.418 -1.507 1.00 24.27 A						86		38.523	15.571	-7.202	1.00 18.57	Α
40 ATOM 129 N ILE A 87 38.737 16.881 -7.227 1.00 17.88 A ATOM 130 CA ILE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 139 CB LEU A 88								39.045	14.807	-6.385	1.00 16.77	А
ATOM 130 CA ILE A 87 39.577 17.554 -6.256 1.00 18.26 A ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A 45 ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 38.815 18.632 -1.901 1.00 23.11 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A ATOM 144 O LEU A 88 38.815 18.632 -1.901 1.00 23.11 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A	40					87		38.737	16.881	-7.227	1.00 17.88	А
ATOM 131 CB ILE A 87 39.994 18.952 -6.772 1.00 19.60 A ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A 45 ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.97 A ATOM 141 CD1 LEU A 88 38.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 38.815 18.632 -1.901 1.00 23.11 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 39.997 19.174 -2.149 1.00 24.27 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 40.367 20.418 -1.507 1.00 25.47											1.00 18.26	A
ATOM 132 CG2 ILE A 87 40.593 19.786 -5.628 1.00 18.73 A ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 143 C LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47					ILE A	87		39.994	18.952	-6.772	1.00 19.60	А
ATOM 133 CG1 ILE A 87 40.968 18.786 -7.945 1.00 21.16 A 45 ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 40.367 20.418 -1.507 1.00 25.47						87			19.786		1.00 18.73	А
45 ATOM 134 CD1 ILE A 87 41.412 20.087 -8.588 1.00 25.26 A ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 40.367 20.418 -1.507 1.00 25.47								40.968		-7.945	1.00 21.16	A
ATOM 135 C ILE A 87 38.731 17.709 -4.997 1.00 19.67 A ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47	45											A
ATOM 136 O ILE A 87 37.628 18.249 -5.052 1.00 20.41 A ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47												
ATOM 137 N LEU A 88 39.240 17.229 -3.867 1.00 19.15 A ATOM 138 CA LEU A 88 38.508 17.324 -2.611 1.00 20.68 A 50 ATOM 139 CB LEU A 88 38.870 16.151 -1.700 1.00 19.97 A ATOM 140 CG LEU A 88 38.529 14.759 -2.237 1.00 19.24 A ATOM 141 CD1 LEU A 88 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47					•							
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ATOM 141 CD1 LEU A 88 . 39.090 13.692 -1.311 1.00 21.41 A ATOM 142 CD2 LEU A 88 37.029 14.622 -2.359 1.00 18.84 A ATOM 143 C LEU A 88 38.815 18.632 -1.901 1.00 23.11 A 55 ATOM 144 O LEU A 88 37.999 19.146 -1.139 1.00 25.10 A ATOM 145 N GLY A 89 39.997 19.174 -2.149 1.00 24.09 A ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47												
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ATOM 146 CA GLY A 89 40.367 20.418 -1.507 1.00 24.27 A ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47 A												
ATOM 147 C GLY A 89 41.658 20.954 -2.078 1.00 25.47 A												

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	MOTA	149	N	GLU	A 9	90	41.870	22.254	-1.906	1.00	26.22	A
	ATOM	150	CA	GLU	A G	90	43.064	22.924	-2.404		29.96	. A
	ATOM	151	СВ	GLU		90	42.698					
								23.814	-3.596		30.75	A
_	MOTA	152	CG	GLΰ		90	42.267	23.038	-4.831		34.32	A
5	ATOM	153	CD	. GLU	A 9	90	41.711	23.930	-5.927	1.00	38.27	Α
	ATOM	154	OE1	GLU	A 9	90	40.590	24.456	-5.764	1.00	40.57	A
	ATOM	155	OE2	GLU	A 9	90	42.398	24.110	-6.952		40.90	A
	ATOM	156	C	GLU		90	43.711	23.768				
									-1.313		30.68	A
	MOTA	157	0	GLU		90	43.049	24.574	-0.668		32.83	A
10	MOTA	158	N	GLY		€1	45.006	23.566	-1.104	1.00	29.66	A
	ATOM	159	CA	\mathtt{GLY}	A 9	91	45.724	24.332	-0.104	1.00	29.40	Α
	ATOM	160	С	GLY	A 9	91	46.795	25.151	-0.798	1.00	29.98	A
	ATOM	161	Ō	GLY		91	46.894		-2.028		28.16	A
	ATOM	162	N	SER		92	47.605					
1								25.870	-0.029		28.30	A
15	ATOM	163	CA	SER		92	48.653	26.681	-0.633	1.00	30.50	A
	MOTA	164	CB	SER	A 9) 2	49.165	27.717	0.370	1.00	32.43	A
	MOTA	165	OG	SER	A 9	92	49.520	27.099	1.593	1.00	40.94	Α
	ATOM	166	С	SER	A 9	92	49.815	25.843	-1.164	1.00	29.77	A
	ATOM	167	0	SER		92	50.456	26.221	-2.143		30.46	A
20		168		PHE		3						
20	ATOM		N				50.087	24.703	-0.536		27.65	A
	ATOM	169	CA	PHE		93	51.185	23.855	-0.995		26.34	A
	ATOM	170	CB	PHE	A 9	3	52.281	23.785	0.068	1.00	27.95	A
	MOTA	171	CG	PHE	A 9	3	52.861	25.117	0.406	1.00	31.06	Α
	ATOM	172	CD1	PHE	A 9	3	52.283	25.909	1.392	1.00	29.96	A
25	ATOM	173		PHE		3	53.949	25.613	-0.308		31.38	A
2.5		174		PHE	_	3	52.779				32.69	
	ATOM							27.181	1.665			A
	ATOM	175		PHE		3	54.452	26.88,3	-0.044		32.63	A
	ATOM -	176	CZ ·	PHE	A 9	3	53.864	27.670	0.945	1.00	31.81	A
	ATOM	177	С	PHE	A 9	3	50.759	22.445	-1.365	1.00	25.39	A
30	ATOM	178	0	PHE	A 9	3	51.601	21.559	-1.522	1.00	24.59	A
	ATOM	179	N	SER		4	49.457	22.235	-1.519		23.63	A
	ATOM	180	CA	SER		4	48.965	20.912	-1.860		21.43	A
	ATOM	181	CB	SER		14	49.017	20.013	-0.628		21.42	A
	ATOM	182	OG	SER		4	48.091	20.475	0.340		21.19	A
35	ATOM	183	С	SER .	A 9	4 .	47.539	20.925	-2.378	1.00	19.82	Α
	ATOM	184	0	SER .	A 9	4	46.795	21.882	-2.173	1.00	18.76	A
	ATOM	185	N	THR	A 9	15	47.174	19.832	-3.038	1.00	19.38	Α
	ATOM	186	CA	THR		5	45.840	19.637	-3.580		17.98	A
	ATOM	187	CB	THR		5	45.818	19.818	-5.110		19.25	A
40 .												
40 ·	ATOM	188		THR .		5	46.196	21.162	-5.434		22.04	A
	MOTA	189		THR .		5	44.421	19.549	-5.661		17.61	A
	ATOM	190	C,	THR .	A 9	5	45.455	18.201	-3.243	1.00	18.61	A
	ATOM	191	0	THR .	A. 9	5	46.212	17.264	-3.524	1.00	17.10	A
	ATOM	192	N	VAL .	A 9	6	44.295	18.024	-2.623	1.00	16.53	A
45	ATOM	193	CA	VAL		6	43.845	16.685	-2.266		16.05	A
	ATOM	194	СВ	VAL		6	43.170	16.672	-0.886		16.32	A
	ATOM	195		VAL .		6	42.741	15.249	-0.532		18.02	A
	ATOM	196	CG2	VAL 2		6	44.145	17.206	0.168		16.69	A
	MOTA	197	С	VAL A	A 9	6	42.875	16.207	-3.335	1.00	16.42	Α
50	ATOM	198	0	VAL 2	A 9	6	41.906	16.892	-3.665	1.00	16.47	A
	ATOM	199	N	VAL I		7	43.157	15.033	-3.888		16.80	A
	ATOM	200	CA	VAL I		7	42.338	14.471	-4.949		16.72	A
	ATOM	201	CB	VAL I		7	43.153	14.354	-6.255		18.43	A
	ATOM	202		VAL A		7	42.249	13.927	-7.404		19.69	A
55	MOTA	203	CG2	VAL I	A 9	7	43.831	15.685	-6.569	1.00	17.84	Α
	ATOM	204	С	VAL Z	A 9	7	41.812	13.091	-4.583	1.00	16.77	A
	ATOM	205	Ō	VAL Z			42.532	12.270	-4.014		17.13	A
	ATOM	206	N	LEU A			40.545	12.845	-4.895		16.62	A
	ATOM	207	CA	LEU A	A 9	U	39.947	11.548	-4.624	1.00	17.04	A

	ATOM	208	СВ				38.424	11.633		1.00 16.89	A
	MOTA	209					37.635	10.342			A
	ATOM	210		1 LEU A			37.990	9.762	-3.146	1.00 20.07	А
_	ATOM	211		2 LEU A			36.143	10.627		1.00 17.93	A
5	ATOM	212	С	LEU A			40.512	10.597		1.00 17.38	A
	ATOM	213	0	LEU A			40.527	10.920		1.00 18.60	A
	ATOM	214	N	ALA A			40.995	9.438		1.00 17.13	A
	ATOM	215	CA				41.570	8.466	-6.168	1.00 18.42	A
10	ATOM	216	CB	ALA A			43.090	8.524	-6.105	1.00 14.76	, A
10	ATOM	217	C	ALA A	99		41.102	7.055		1.00 21.40	A
	ATOM	218	0	ALA A			40.941	6.691	-4.679	1.00 22.52	A
	ATOM	219	N	ARG A			40.878	6.261	-6.888	1.00 19.77	A
	ATOM	220	CA	ARG A			40.459	4.884	-6.693	1.00 20.85	A
15	ATOM	221	CB	ARG A			39.202	4.585	-7.518	1.00 24.22	A
15	MOTA	222	CG	ARG A			38.608	3.205	-7.256	1.00 31.78	A
	ATOM ATOM	223	CD	ARG A			37.326	2.979	-8.048	1.00 36.24	A
	ATOM	224 225	NE	ARG A			36.213	3.818	-7.594	1.00 41.40	A
	ATOM	225	CZ	ARG A			35.566	3.662	-6.439	1.00 42.05	
20	ATOM	227		L ARG A			35.912	2.696	-5.598	1.00 40.67	Α
20	ATOM	228	C	ARG A		!	34.559	4.468	-6.128	1.00 43.65	A
	ATOM	229	Ö	ARG A			41.613 42.078	3.985 4.065	-7.129	1.00 18.63	A
	ATOM	230	N	GLU A			42.078		-8.271	1.00 19.49	A
	ATOM	231	CA	GLU A			43.196	3.157 2.246	-6.212 -6.533	1.00 16.43	A
25	ATOM	232	CB	GLU A			43.774	1.637	-5.248	1.00 16.11 1.00 16.79	A
20	ATOM	233	CG	GLU A			44.917	0.657	-5.488	1.00 16.79	A A
	ATOM	234	CD	GLU A			45.501	0.115	-4.200	1.00 18.20	A
	ATOM	235		GLU A			44.733	-0.081	-3.239	1.00 18.20	A
	ATOM	236		GLU A			46.725	-0.132	-4.150	1.00 10.32	A
30	ATOM`	237	C	GLU A			42.625	1.152	-7.442	1.00 17.14	A
	ATOM	238	0	GLU A			41.681	0.462	-7.069	1.00 18.02	. A
	ATOM	239	N.	LEU A			43.198	1.002	-8.632	1.00 19.06	A
	ATOM	240	CA	LEU A	102		42.718	0.025	-9.607	1.00 20.71	A
	ATOM	241	CB	LEU A	102		43.569		-10.878	1.00 23.42	A
35	ATOM	242	CG	LEU A	102		43.531	1.426	-11.642	1.00 25.30	A
	ATOM	243		LEU A			44.577	1.414	-12.748	1.00 27.88	Α
	ATOM	244	CD2	LEU A	102		42.140	1.647	-12.214	1.00 26.79	A
	ATOM	245	С	LEU A			42.671	-1.418	-9.125	1.00 21.62	Α
	MOTA	246	0	LEU A	102		41.668	-2.103	-9.305	1.00 21.09	A
40	MOTA	247	N	ALA A			43.753	-1.874	-8.507	1.00 19.38	A
	MOTA	248	CA	ALA A			43.836	-3.249	-8.035	1.00 20.87	A
	ATOM	249	CB	ALA A			45.284	-3.571	-7.671	1.00 19.23	A
	ATOM	250	С	ALA A			42.919	-3.629	-6.872	1.00 19.92	А
4.5	ATOM	251	0	ALA A			42.703	-4.815	-6.628	1.00 20.38	Α
45	ATOM	252	Ŋ	THR A			42.361	-2.643	-6.175	1.00 18.12	A
	ATOM	253	CA	THR A			41.517	-2.927	-5.018	1.00 17.15	Α
	ATOM	254	CB	THR A			42.212	-2.484	-3.717	1.00 19.54	A
	ATOM	255		THR A			42.456	-1.070	-3.773	1.00 19.26	A
50	ATOM	256		THR A			43.536	-3.219	-3.529	1.00 17.02	A
50	ATOM	257	C	THR A			40.159	-2.247	-5.026	1.00 19.44	A
	ATOM	258	0 .	THR A			39.259	-2.648	-4.285	1.00 18.70	A
	ATOM	259	N Ch	SER A			40.034	-1.207	-5.847	1.00 19.65	A
	ATOM	260	CA	SER A			38.819	-0.400	-5.967	1.00 19.37	A
55	ATOM ATOM	261 262	CB .	SER A			37.598	-1.304	-6.173	1.00 21.81	A
<i></i>	ATOM	263	OG C	SER A SER A			36.431 38.644	-0.539	-6.412	1.00 23.01	A
	ATOM	264	0	SER A			37.602	0.447 1.070	-4.701 -4.400	1.00 18.99	A
	ATOM	265	Ŋ	ARG A			39.674	0.468	-4.488 -3.961	1.00 18.66 1.00 16.84	À
	ATOM	266	CA	ARG A			39.655		-3.861 -2.634	1.00 16.84	A.
	-11-013	200	U.A	א טייני	±00 .			1.267	-2.034	T.00 TO.21	Α

	ATOM	267	CB	ARG	Α	106		40.827	0.886	-1.723	1.00 16.41	A
	MOTA	268	CG	ARG	Α	106		40.619	-0.367	-0.906	1.00 15.49	A
	ATOM	269	CD	ARG	Α	106		41.887	-0.755	-0.170	1.00 17.43	Α
	ATOM	270	NE	ARG	Α	106		41.620	-1.792	0.824	1.00 20.47	A
5 '	MOTA	271	CZ	ARG	A	106		42.548	-2.568	1.371	1.00 20.24	A
	ATOM	272	NH1	ARG	Α	106		43.821	-2.433	1.017	1.00 17.80	A
	ATOM	273	NH2	ARG	Α	106		42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG	Α	106		39.785	2.746	-2.981	1.00 17.37	A
	ATOM	275	0	ARG				40.514	3.103	-3.902	1.00 17.75	A
10	ATOM	276	N	GLU				39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU				39.156	5.039	-2.461	1.00 20.80	A
	ATOM	278	СВ	GLU				37.779	5.694	-2.337	1.00 22.93	A
•	ATOM	279	CG	GLU				36.711	5.171	-3.269	1.00 30.87	A
	ATOM	280	CD	GLU				35.431	5.975	-3.148	1.00 32.40	A
15	ATOM	281	OE1					35.262	6.939	-3.923	1.00 32.74	A
10	ATOM	282	OE2					34.608	5.654	-2.263	1.00 35.74	A
	ATOM	283	C	GLU				40.053	5.678	-1.410	1.00 30.00	A
	ATOM	284	Ö	GLU			•	39.891	5.427	-0.220	1.00 10.33	A
	ATOM	285	N	TYR				40.988	6.507	-1.852	1.00 15.21	Ā
20	ATOM	286	CA	TYR				41.883	7.209	-0.942	1.00 15.86	· A
20	ATOM	287	CB	TYR				43.325	6.728	-1.104	1.00 15.30	A
	ATOM	288	CG	TYR				43.523	5.328	-0.612	1.00 15.30	A
	ATOM	289		TYR				43.765	5.066	0.746	1.00 16.35	A
		290	CE1	TYR				44.046	3.769	1.201	1.00 18.38	. A
25	ATOM ATOM	290	CD2	TYR				43.701	4.268	-1.511	1.00 13.45	A
23		292	CE2					43.701	2.981	-1.075	1.00 13.23	A
	ATOM ATOM	293	CZ	TYR				44.152	2.736	0.276	1.00 17.20	A
	ATOM	294	OH	TYR				44.440	1.461	0.688	1.00 19.17	A
	ATOM	295	C	TYR				41.850	8.687	-1.292	1.00 15.30	A
30		296	0	TYR				41.560	9.058	-2.431	1.00 15.22	A
30	ATOM	290 297	N	ALA				42.132	9.528	-0.306	1.00 13.22	A
	ATOM ATOM	298	CA	ALA				42.132	10.957	-0.539	1.00 14.30	A
		299	CB	ALA				41.671	11.726	0.661	1.00 14.78	A
	ATOM	300	СБ	ALA				43.713	11.136	-0.667	1.00 14.70	· A
35	ATOM ATOM	301	0	ALA				44.450	10.983	0.317	1.00 16.73	A
33		302	N	ILE				44.182	11.410	-1.881	1.00 10.32	.A
	MOTA	302	CA	ILE				45.609	11.574	-2.093	1.00 15.80	A.
	ATOM ATOM	303	CB	ILE				46.065	10.863	-3.396	1.00 15.00	A
		305	CG2	ILE				47.550	11.098	-3.632	1.00 16.80	A
40	ATOM ATOM	305	CG1	ILE				45.774	9.358	-3.032	1.00 10.00	A
40	ATOM	307	CD1					46.308	8.513	-4.437	1.00 17.70	A
	ATOM	308	CDI	ILE				46.004	13.045	-2.129	1.00 17.78	A
	ATOM	309	0	ILE				45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS				46.846	13.435	-1.177	1.00 16.24	A
45		311	-	LYS				47.326	14.808	-1.100	1.00 17.20	A
43	ATOM ATOM	312	CA CB	LYS				47.700	15.176	0.344	1.00 17.20	A
	ATOM	313	CG	LYS				48.350	16.547	0.464	1.00 17.41	A
		314	CD	LYS				48.585	16.971	1.910	1.00 24.25	A
	ATOM ATOM	315	CE	LYS				47.288	17.381	2.598	1.00 24.25	A
50	ATOM	316	NZ	LYS				47.516	17.866	4.000	1.00 20.40	A
50		317		LYS				48.551	14.890	-1.994	1.00 16.41	A
	ATOM ATOM	318	C	LYS				49.509	14.137	-1.813	1.00 10.41	A.
			0					48.509	15.798	-2.963	1.00 15.20	A
	ATOM	319	N	ILE ILE				49.606	15.798	-2.963	1.00 13.87	A
55	ATOM	320	CA CB	ILE				49.006	15.967	-5.358	1.00 17.28	A
در	ATOM	321		ILE				50.235	15.911	-6.341	1.00 15.43	A
	ATOM	322		ILE				48.293	14.609	-5.565	1.00 15.12	A
	ATOM	323		ILE				47.580	14.509	-6.904	1.00 18.82	A
	ATOM	324	CDI	ILE				50.307	17.301	-3.663	1.00 19.03	A
	ATOM	325	C	TUD	~	442		50.307	11.301	5.005	2.00 15.05	

	. ATOM	326	0	ILE A 11:	2 49.669	.18.350	-3.635	1.00 19.15	A
	ATOM	327	N	LEU A 11:		17.245	-3.472	1.00 20.22	, A
	ATOM	328	CA	LEU A 11:		18.442	-3.214	1.00 22.36	. A
	ATOM	329	СВ	LEU A 11:		18.397	-1.794	1.00 22.13	. A
5	ATOM	330	CG	LEU A 113		18.063	-0.646	1.00 22.46	A
	ATOM	331	CD1	L LEU A 113		16.557	-0.553	1.00 23.81	A
	ATOM	332	CD2	2 LEU A 113		18.595	0.660	1.00 23.68	A
	ATOM	333	С	LEU A 113		18.547	-4.215	1.00 23.37	A
	ATOM	334	0	LEU A 113	3 54.300	17.586	-4.424	1.00 23.11	A
10	ATOM	335	N	GLU A 114		19.714	-4.834	1.00 23.88	A
	ATOM	336	CA	GLU A 114		19.920	-5.806	1.00 26.00	A
	ATOM	337	CB	GLU A 114		21.111	-6.706	1.00 27.74	A
	ATOM	338	CG	GLU A 114	4 55.533	21.452	-7.696	1.00 35.07	A
	ATOM	339	CD	GLU A 114	4 55.220	22.696	-8.497	1.00 39.24	A
15	ATOM	340	OE1	GLU A 114	4 54.808	23.703	-7.885	1.00 41.45	A
	ATOM	341	OE2	GLU A 114	4 55.395	22.670	-9.736	1.00 44.05	A
	ATOM	342	С	GLU A 114	4 56.087	20.163	-5.067	1.00 24.37	A
	ATOM	343	0	GLU A 114	56.186	21.071	-4.238	1.00 24.43	A
	MOTA	344	N	LYS A 115	57.096	19.350	-5.360	1.00 24.10	A
20	ATOM	345	CA	LYS A 115	58.376	19.493	-4.678	1.00 24.93	A
	MOTA	346	CB	LYS A 115	5 59.339	18.373	-5.103	1.00 23.72	Α
	ATOM	347	CG	LYS A 115	5 59.139	17.080	-4.308	1.00 23.09	A
	ATOM	348	CD	LYS A 115	60.064	15.944	-4.743	1.00 21.92	A
	ATOM	349	CE	LYS A 115	59.691	15.400	-6.117	1.00 22.42	A
25	ATOM	350	NZ	LYS A 115		14.150	-6.448	1.00 19.71	A
	ATOM	351	С	LYS A 115	59.031	20.858	-4.868	1.00 26.87	A
	ATOM	352	0	LYS A 115		21.469	-3.903	1.00 26.17	A
	MOTA	353	N	ARG A 116	59.058	21.348	-6.102	1.00 28.73	A
	MOTA	354	CA	ARG A 116	5 . 59.678	22.638	-6.380	1.00 29.66	A
30	ATOM	355	СВ	ARG A 116		22.980	-7.868	1.00 31.29	Α
	ATOM	356	CG	ARG A 116		24.361	-8.267	1.00 33.19	A
	ATOM	357	CD	ARG A 116		24.710	-7.590	1.00 35.13	A
	ATOM	358	ΝE	ARG A 116		23.612	-7.618	1.00 36.42	А
	ATOM	359	CZ	ARG A 116		23.648	-7.009	1.00 36.18	A
35	ATOM	360		ARG A 116		24.729	-6.332	1.00 36.12	A
	ATOM	361		ARG.A 116		22.602	-7.067	1.00 35.77	Α
	ATOM .	362	C	ARG A 116		23.761	-5.519	1.00 29.70	A
	ATOM	363	0	ARG A 116		24.515	-4.889	1.00 29.16	Α
40	ATOM	364	N	HIS A 117		23.862	-5.472	1.00 27.22	A
40	ATOM	365	CA	HIS A 117		24.903	-4.681	1.00 26.33	A
	ATOM	366	CB	HIS A 117		24.835	-4.848	1.00 28.41	A
	ATOM ATOM	367	CG	HIS A 117		26.005	-4.258	1.00 31.82	A
		368		HIS A 117		27.249	-3.935	1.00 33.19	A
45	ATOM ATOM	369 370		HIS A 117		25.974	-3.961	1.00 34.30	A
40			CEI	HIS A 117	53.165	27.148	-3.480	1.00 34.58	A
•	ATOM ATOM	371		HIS A 117		27.940	-3.455	1.00 35.18	A
	ATOM	372 373	С	HIS A 117		24.780	-3.202	1.00 26.22	A
	ATOM	374	O N	HIS A 117 ILE A 118		25.776	-2.534	1.00 25.67	A
50	ATOM	375	CA			23.554	-2.689	1.00 24.94	A
50	ATOM	376	CB	ILE A 118 ILE A 118		23.315 21.812	-1.285	1.00 23.94	A
	ATOM	377		ILE A 118			-0.952	1.00 23.50	A
	ATOM	378		ILE A 118		21.533	0.389	1.00 23.76	A
	ATOM	379		ILE A 118		21.362 19.858	-0.959 -0.834	1.00 24.42 1.00 28.06	A
55	ATOM	380	CDI	ILE A 118	59.195	23.821	-0.834 -0.958	1.00 28.06	A
	ATOM	381	0	ILE A 118	59.402	24.495	0.048	1.00 23.78	A n
	ATOM	382	N	ILE A 119		23.489	-1.815	1.00 23.49	A
	ATOM	383	CA	ILE A 119		23.469	-1.619	1.00 25.46	A À
•	ATOM	384	CB	ILE A 119	62.467	23.250	-2.664	1.00 23.13	A A
				43 3.13	02.4707		£ . 004	T.OO 74.73	n

					_			•				•
-	ATOM	385		2 ILE P			63.858	23.890	-2.617	1.00 2	2.47	A
	MOTA	386		1 ILE A			62.540	21.738	-2.395			A
	MOTA	387	CD:	1 ILE A	119		63.327	20.945	-3.439			A
	ATOM	388		ILE A	119		61.667	25.435	-1.705			A
5	ATOM	389	0	ILE A	119		62.330	26.051	-0.872	1.00 2		A
	MOTA	390) N	LYS A	120		61.028		-2.704	1.00 2		A
	ATOM	391	. CA	LYS A	120		61.100	27.489	-2.879	1.00 3		A
	ATOM	392	CB	LYS A	120		60.242		-4.060	1.00 3		A
	ATOM	393	CG	LYS A	120		60.674		-5.409	1.00 3		A
10	ATOM	394	CD	LYS A	120		59.765		-6.512	1.00 4		A
	ATOM	395	CE	LYS A	120		58.294		-6.218	1.00 4		A
	ATOM	396	NZ	LYS A	120		57.363		-7.252	1.00 4		A
	ATOM	397	С	LYS A	120		60.647		-1.638	1.00 3		A
	ATOM	398	0	LYS A	120		61.303		-1.217	1.00 3		A
15	ATOM	399	N	GLU A	121		59.527		-1.055	1.00 2		A
	ATOM	400	CA	GLU A			58.986		0.128	1.00 2		A
	ATOM	401	СВ	GLU A			57.455	28.416	0.117	1.00 3		A
	ATOM	402	CG	GLU A			56.794	29.021	-1.120	1.00 3		A
	ATOM	403		GLU A			57.221	30.456	-1.373	1.00 3		A
20	ATOM	404	OE1	GLU A			57.200	31.264	-0.420	1.00 40		A
	ATOM	405					57.573	30.778	-2.529	1.00 43		
	ATOM	406		GLU A			9.511	27.930	1.451	1.00 4.		A
	ATOM	407	0	GLU A			8.946	28.204	2.513	1.00 3		, A A
	ATOM ·	408	N	ASN A			50.588	27.151	1.390	1.00 3		A
25	ATOM	409	CA	ASN A			51.183	26.573	2.594	1.00 28		A
	ATOM	410	СВ	ASN A			1.836	27.673	3.436	1.00 20		
	ATOM	411	CG	ASN A			2.945	28.395	2.698	1.00 34		A
	ATOM	412		ASN A			2.697	29.143	1.754	1.00 35		A
	ATOM	413		ASN A			4.181	28.169	3.127	1.00 35		A
30	ATOM	414	С	ASN A			0.157	25.835	3.456	1.00 26		A
	ATOM	415	ō	ASN A			0.085	26.055	4.663	1.00 27		A
	ATOM	416	N	LYS A			9.375	24.955	2.842	1.00 27		A
	ATOM	417	CA	LYS A			8.358	24.210	3.574	1.00 23		A
	ATOM	418	СВ	LYS A			7.031	24.248	2.810	1.00 22		A
35	ATOM	419	CG	LYS A			6.475	25.645	2.599			A
	ATOM	420	CD	LYS A			6.253	26.354	3.927	1.00 23		A
	ATOM	421	CE	LYS A			5.822	27.796	3.716			A
	ATOM	422	NZ	LYS A			5.756	28.540	5.004	1.00 31 1.00 33		A
	ATOM	423	C	LYS A			8.748	22.759	3.821			A
40	ATOM	424	ō	LYS A			7.924	21.960	4.264	1.00 22 1.00 22		. A
	ATOM	425	N	VAL A			9.997	22.412	3.535	1.00 22		A
•	ATOM	426	CA	VAL A			0.439	21.039	3.730	1.00 20		A
	ATOM	427	СВ	VAL A			1.922	20.850	3.730	1.00 20		A
	ATOM	428		VAL A			2.346	19.407	3.573			A
45	ATOM	429		VAL A		_				1.00 18		A
	ATOM	430	C	VAL A			2.104 0.236	21.195 20.561	1.853	1.00 18		A
	ATOM	431	Ö	VAL A			9.841	19.418	5.163	1.00 19		A
	ATOM	432	N	PRO A			0.513		5.385	1.00 20		A
	ATOM	433	CD	PRO A			1.178	21.422 22.738	6.159	1.00 20		A
50	ATOM	434	CA	PRO A			0.318		6.118	1.00 18		A
	ATOM	435	CB	PRO A				20.979	7.544	1.00 19		A
	ATOM	436	CG	PRO A			0.793	22.180	8.363	1.00 19		A
	ATOM	437	C	PRO A			L.839	22.805	7.479	1.00 18		A
	ATOM	437	0				3.848	20.642	7.824	1.00 19		A
55	ATOM	438	N	PRO A			3.544	19.700	8.550	1.00 16		A
23	ATOM	439		TYR A			7.947	21.418	7.235	1.00 18		Α
	ATOM	441	CA CB	TYR A			5.516	21.220	7.435	1.00 21		A
	ATOM	441		TYR A			752	22.448	6.933	1.00 25		A
				TYR A			5.040	23.690	7.748	1.00 30		A
	ATOM	443	CD1	TYR A	126	55	.438	23.886	8.991	1.00 33	. 95	A

								•		• •	• • •	
	ATOM	444		LTYR				55.721	25.015	9.763	1.00 36.60	A
	ATOM	445		YYP			-	56.938	24.657	7.292	1.00 35.43	Ā
	ATOM	446	CE	YYR	A	126		57.231	25.792	8.058	1.00 37.20	· :•· A
	ATOM	447	CZ			126		56.618	25.962	9.291	1.00 37.40	A
5	ATOM	448	ОН	TYR	A	126		56.903	27.073	10.052	1.00 40.85	A
	MOTA	449	С	TYR	A	126		55.990	19.956	6.762	1.00 21.35	A
	MOTA	450	0	TYR	A	126		55.265	19.175	7.383	1.00 20.49	A
	ATOM	451	N	VAL	Α	127		56.354	19.746	5.501	1.00 18.16	A
	ATOM	452	CA	VAL	Α	127		55.892	18.562	4.790	1.00 17.58	A
10	ATOM	453	CB	VAL	Α	127		56.308	18.596	3.308	1.00 17.45	A
	ATOM	454		VAL				55.786	17.350	2.600	1.00 17.97	A
	ATOM	455	CG2					55.751	19.850	2.641	1.00 14.90	A
	. ATOM	456	С			127		56.459	17.306	5.448	1.00 18.39	A
	ATOM	457	0	VAL	Α	127		55.769	16.298	5.583	1.00 18.14	A
15	MOTA	458	N			128		57.716	17.381	5.869	1.00 17.50	A
	ATOM	459	CA	THR	Α	128		58.375	16.260	6.530	1.00 18.54	A
	MOTA	460	СВ			128		59.861	16.586	6.805	1.00 18.01	A
	ATOM	461	OG1	THR				60.537	16.804	5.559	1.00 21.14	A
	ATOM	462	CG2	THR	Α	128		60.536	15.446	7.545	1.00 17.95	Α
20	ATOM	463	C			128		57.676	15.941	7.856	1.00 19.49	Α
	ATOM	464	0			128		57.438	14.776	8.179	1.00 18.76	Α
	ATOM	465	N			129		57.345	16.981	8.619	1.00 19.60	A
	MOTA	466	CA			129		56.673	16.804	9.904	1.00 20.12	Α
	MOTA	467	CB			129		56.534	18.144	10.621	1.00 21.33	A
25	ATOM	468	CG			129		55.948	18.029	12.023	1.00 28.02	A
	ATOM	469	CD			129		55.721	19.404	12.597	1.00 31.25	Α
	ATOM	470	NE			129		56.940	20.205	12.560	1.00 37.78	A
	ATOM	471	CZ			129		56.962	21.524	12.391	1.00 40.10	A
20	ATOM	472		ARG				55.828	22.197	12.239	1.00 40.03	A
30	ATOM	473		ARG				58.119	22.170	12.374	1.00 44.58	A
	ATOM	474	C			129		55.288	16.186	9.729	1.00 20.08	A
	ATOM ATOM	475 476	N O			129 130		54.891	15.305	10.496	1.00 20.40	A
	ATOM	477	CA			130		54.553 53.222	16.654 16.125	8.724 8.454	1.00 18.79 1.00 20.10	A A
35	ATOM	478	CB			130		52.638	16.749	7.183	1.00 20.10	A
55	ATOM	479	CG	GLU				51.350	16.087	6.708	1.00 13.32	A A
	ATOM	480	CD			130		50.581	16.933	5.707	1.00 27.83	A
	ATOM	481	OE1					51.216	17.528	4.814	1.00 23.72	A
	ATOM	482		GLU				49.339	16.996	5.807	1.00 30.74	A
40	MOTA	483	C			130		53.301	14.615	8.295	1.00 19.81	A
	ATOM	484	ō	GLU				52.553	13.875	8.935	1.00 18.37	A
	ATOM	485	N	ARG				54.219	14.162	7.447	1.00 20.41	A
	ATOM	486	CA	ARG				54.397	12.735	7.202	1.00 22.45	A
	ATOM	487	CB	ARG	Α	131		55.442	12.511	6.098	1.00 25.16	A
45	ATOM	488	CG	ARG	Α	131		55.742	11.043	5.840	1.00 28.75	A
	ATOM	489	CD	ARG				56.736	10.837	4.708	1.00 33.75	A
	ATOM	490	NE	ARG				57.020	9.415	4.520	1.00 40.07	Α
	ATOM	491	CZ	ARG	Α	131		57.756	8.915	3.532	1.00 43.07	A
	ATOM	492	NH1	ARG	Α	131		58.293	9.721	2.625	1.00 44.91	Α
50	ATOM	493	NH2	ARG	Α	131		57.955	7.606	3.449	1.00 44.45	A
	ATOM	494	С	ARG	A	131		54.820	11.982	8.466	1.00 23.24	A
	MOTA	495	0	ARG				54.241	10.948	8.804	1.00 23.86	Α
	ATOM	496	N	ASP				55.831	12.497	9.160	1.00 21.99	A
	ATOM	497	CA	ASP				56.318	11.850.	10.370	1.00 22.04	Α
55	ATOM	498	CB	ASP				57.570	12.564	10.888		. А
	MOTA		CG	ASP				58.750	12.442	9.932	1.00 27.77	Α
	ATOM	500		ASP				58.681	11.620	8.989	1.00 27.34	A
	ATOM	501		ASP				59.753	13.163	10.128	1.00 28.70	A
	ATOM	502	С	ASP	A	132		55.258	11.772	11.474	1.00 21.69	A

	ATOM	503	0	ASP	А	132		55.077	10.723	12.092	1.00	22.75		Α
	ATOM	504	N	VAL	Α	133	•	54.551	12.868	11.725		19.54	•	Α
	ATOM	505	CA			133		53.525	12.843	12.759		18.52		Α
	ATOM	506	CB			133		52.908	14.244	12.990		19.26		Α
5	ATOM	507		VAL				51.708	14.135	13.918		18.79		Α
-	ATOM	508		VAL				53.953	15.180	13.604		18.80		A
	ATOM	509	C	VAL				52.419	11.854	12.398		19.46		A
	ATOM	510	o	VAL				52.419	10.991	13.200		19.40		
	ATOM	511	N	MET										A
10								51.878	11.957	11.187		19.15		A
10	ATOM	512	CA	MET				50.807	11.052	10.792		21.25		A
	ATOM	513	CB	MET				50.309	11.381	9.383		17.34		A
	ATOM	514	CG	MET				49.615	12.730	9.302		20.00		A
	ATOM	515	SD			134"		48.643	12.952	7.798		24.21		A
٠. ـ	ATOM	516	CE	MET			•	47.033	12.434	8.400		23.20		A
15	ATOM	517	С	MET				51.203	9.582	10.881		22.43		A
	ATOM	518	0	MET				50.384	8.741	11.249		23.82		Α
	ATOM	519	N	SER	Α	135		52.454	9.273	10.556	1.00	23.09		A
	ATOM	520	CA	SER	Α	135		52.939	7.895	10.615	1.00	26.13		Α
	ATOM	521	CB	SER	Α	135		54.356	7.798	10.039	1.00	26.17		Α
20	ATOM	522	OG	SER	Α	135		54.383	8.177	8.673	1.00	31.91		Α
	ATOM	523	C	SER	Α	135		52.957	7.358	12.045	1.00	26.58		Α
	ATOM	524	0	SER	А	135		52.926	6.148	12.261	1.00	26.42		Α
	ATOM	525	N	ARG	A	136		53.014	8.261	13.018	1.00	25.65		Α
	ATOM	526	CA	ARG				53.056	7.870	14.425	1.00	27.47		Α
25	ATOM	527	СВ	ARG	Α	136		53.823	8.914	15.238	1.00	27.97		Α
	ATOM	528	CG	ARG				55.283	9.082	14.857		32.00		A
	ATOM	529	CD	ARG				55.904	10.218	15.664		33.03		A
	ATOM	530	NE	ARG				55.602	10.073	17.084		36.11		A
•	ATOM	531	CZ	ARG				55.867	10.990	18.007		39.74		A
30	ATOM	532		ARG				56.449	12.132	17.661		40.55		A
50	ATOM	533		ARG				55.540	10.769	19.276		36.72		A
	ATOM	534	C	ARG				51.667	7.709	15.036		26.38		A
		535						51.516	7.121	16.106		27.06		Α
	ATOM	536	0	ARG				50.655	8.235	14.360		24.77		A
25	MOTA		N	LEU				49.294	8.162	14.870		24.70		A.
35	ATOM	537	CA	LEU								24.70		A.
	ATOM	538	CB	LEU				48.483	9.363	14.371				
	MOTA	539	CG	LEU				49.050	10.760	14.662		26.67		A
	ATOM	540		LEU				48.075	11.813	14.141		27.25		A
40	ATOM	541		LEU				49.279	10.945	16.155		27.09		A
40	ATOM	542	C	LEU				48.592	6.868	14.473		25.20		A
	MOTA	543	0	LEU				48.619	6.469	13.309		25.99		A
	ATOM	544	N	ASP				47.971	6.218	15.451		21.89		A
	ATOM	545	CA	ASP				47.239	4.977	15.219		21.35		A
	ATOM	546	CB	ASP	А	138		48.124	3.761	15.523		22.14		A
45	ATOM	547	CG	ASP				47.432	2.448	15.201		24.90		A
	MOTA	548		ASP				46.631	2.423	14.241		24.78		Α
	MOTA	549	OD2	ASP	Α	138		47.691	1.443	15.897		25,39		Α
	ATOM	550	С	ASP	Α	138		46.031	4.991	16.138	1.00	20.47		Α
	MOTA	551	0	ASP	Α	138		45.967	4.248	17.118		19.06		A
50	MOTA	552	N	HIS	Α	139		45.075	5.852	15.810	1.00	18.27	·	. A
	ATOM	553	CA	HIS	Α	139		43.869	6.016	16.606	1.00	18.21		Α
	MOTA	554	CB	HIS	Α	139		44.096	7.157	17.612	1.00	15.84		Α
	ATOM	555	CG	HIS				42.985	7.332	18.600	1.00	15.24	•	Α
	ATOM	556		HIS				42.884	6.964	19.900		13.97		Α
55	ATOM	557		HIS				41.791	7.943	18.280	1.00	14.74		A
	ATOM	558		HIS				41.002	7.944	19.341		14.19		Α
	ATOM	559		HIS				41.641	7.356	20.336		14.15		A
	ATOM	560	C	HIS				42.715	6.330	15.654		18.50		
	ATOM	561	Ō	HIS				42.879	7.080	14.693		20.80		A A

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	ATOM	562	N	PRO 2	A 140		41.527	5.767	15.913	1.00 18.32	А
	ATOM	563	CD		A 140		41.143	4.984	17.100	1.00 16.71	
	ATOM	564	CA		A 140		40.367	6.001			A
	ATOM	565	CB						15.048	1.00 17.43	Α
•					A 140		39.273	5.157	15.704	1.00 16.64	A
5	ATOM	566	CG		A 140		39.643	5.204	17.152	1.00 18.43	Α
	ATOM	567	С		4 140		39.914	7.441	14.803	1.00 18.77	A
	ATOM	568	0	PRO A	A 140		39.207	7.695	13.831	1.00 19.88	Α
	ATOM	569	N	PHE A	A 141		40.301	8.381	15.664	1.00 17.14	A
	ATOM	570	CA	PHE 2	A 141		39.874	9.767	15.477	1.00 16.42	A
10	ATOM	571	CB	PHE A	A 141		39.568	10.422	16.836	1.00 14.60	A
	ATOM	572	CG		141		38.386	9.817	17.556	1.00 14.00	A
	ATOM	573		PHE A			37.335	9.234	16.842		
										1.00 14.78	A
	ATOM	574		PHE A		•	38.297	9.880	18.942	1.00 13.70	A
1.5	ATOM	575		PHE A			36.215	8.727	17.502	1.00 16.94	A
15	ATOM	576		PHE A			37.178	9.375	19.615	1.00 15.75	Α
	ATOM	577	CZ	PHE A	141		36.135	8.799	18.893	1.00 16.89	A
	ATOM	578	С	PHE A	141		40.857	10.641	14.694	1.00 16.15	Α
	ATOM	579	0	PHE A	141		40.799	11.871	14.761	1.00 17.35	А
	ATOM	580	N	PHE A	142		41.748	10.011	13.941	1.00 15.88	A
20	ATOM	581	ĊA	PHE A			42.727	10.756	13.154	1.00 17.89	A
	ATOM	582	СВ	PHE A			44.115	10.645	13.793	1.00 17.57	A
	ATOM	583	CG	PHE F			44.240	11.371			
									15.103	1.00 18.74	A
	ATOM	584		PHE A			44.559	12.726	15.135	1.00 17.77	A
	ATOM	585		PHE F			43.997	10.711	16.304	1.00 18.74	A
25	ATOM	586		PHE A			44.632	13.417	16.347	1.00 15.77	A
	ATOM	587		PHE F	142		44.065	11.393	17.522	1.00 17.56	A
	ATOM	588	CZ	PHE F	142		44.383	12.747	17.542	1.00 17.14	A
	MOTA	589	С	PHE A	142		42.793	10.231	11.729	1.00 19.12	Α
	ATOM	590	0	PHE A	142		42.659	9.030	11.504	1.00 20.01	A
30	ATOM	591	N	VAL F			42.978	11.135	10.769	1.00 18.72	A
	ATOM	592	CA	VAL A			43.102	10.735	9.371	1.00 18.52	A
	ATOM	593	СВ	VAL A			43.294	11.961	8.440	1.00 20.66	A
	ATOM	594		VAL A			43.843	11.521	7.080	1.00 20.00	A
25	MOTA	595		VAL A			41.958	12.673	8.252	1.00 22.97	A
35	ATOM	596	С	VAL A			44.342	9.865	9.330	1.00 18.68	A
	ATOM	597	0	VAL A			45.355	10.199	9.943	1.00 18.42	A
	ATOM	598	N	LYS A	144		44.259	8.745	8.623	1.00 18.30	A
	ATOM	599	CA	LYS A	144		45.384	7.824	8.535	1.00 18.78	A
•	ATOM	600	CB	LYS A	144		44.889	6.373	8.608	1.00 22.27	A
40	ATOM	601	CG	LYS A	144		46.017	5.340	8.557	1.00 29.72	A
	ATOM	602	CD	LYS A	144		45.491	3.912	8.674	1.00 34.16	A
	ATOM	603	CE	LYS A			46.631	2.896	8.577	1.00 37.67	A
		604	NZ	LYS A				1.484	8.629	1.00 39.02	A
	ATOM	605	C	LYS A			46.192	8.002	7.261	1.00 18.53	A
45		606	_								_
73	ATOM		0	LYS A			45.643	8.314	6.200	1.00 18.18	A
	ATOM	607	N	LEU A			47.502	7.816	7.385	1.00 16.79	A
	ATOM	608	CA	LEU A			48.411	7.900	6.251	1.00 17.45	A
	ATOM	609	CB	LEU A			49.686	8.653	6.641	1.00 18.82	A
	ATOM	610	CG	LEU A	145		50.734	8.902	5.549	1.00 20.23	A
50	ATOM	611	CD1	LEU A	145		51.836	9.799	6.093	1.00 18.83	A
	ATOM	612	CD2	LEU A	145		51.317	7.581	5.069	1.00 19.79	A
	ATOM	613	С	LEU A			48.739	6.450	5.907	1.00 19.19	Α
	ATOM	614	ō	LEU A			49.451	5.772	6.659	1.00 17.36	A
	ATOM	615	N	TYR A			48.215	5.972	4.782	1.00 17.30	A
55	ATOM	616	CA	TYR A			48.444	4.593	4.358	1.00 17.20	A
J.J				TYR A							
	ATOM	617	CB				47.288	4.098	3.486	1.00 17.74	A
	ATOM	618	CG	TYR A			45.981	3.926	4.214	1.00 17.50	A
	ATOM	619		TYR A			45.099	4.995	4.377	1.00 16.50	Α
	ATOM	620	CE1	TYR A	146		43.881	4.827	5.039	1.00 17.10	A

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	ATOM	621	CD2 TY	TR A 146	45.620	2.686	4.735	1.00 18.28	А
	ATOM	622		(R A 146		•			A A
	ATOM	623	CZ TY	R A 146	43.547			1.00 17.53	A
	ATOM	624	OH TY	R A 146	42.342		6.169	1.00 17.55	
5	ATOM	625	C TY	R A 146	49.735		3.582	1.00 20.07	A
	ATOM	626		R A 146	50.382		3.715	1.00 18.72	A
	ATOM	627		IE A 147	50.110		2.765		A
	ATOM	628		E A 147	51.307	5.203	1.952	1.00 18.09	A
	ATOM	629		IE A 147	51.007	4.258	0.783	1.00 17.20	A
10	ATOM	630		E A 147	49.835	4.699	-0.070	1.00 16.77	A
	ATOM	631		E A 147	49.967	5.752	-0.975	1.00 17.75	A
	MOTA	632		E A 147	48.595	4.075	0.053	1.00 16.58	A
	ATOM	633		E A 147	48.886	6.178	-1.742	1.00 18.07	A
	ATOM	634		E A 147	47.503	4.492	-0.710	1.00 19.62	A
15	ATOM	635		E A 147	47.647	5.546	-1.610	1.00 18.56	A
	ATOM	636		E A 147	51.768	6.533	1.395	1.00 19.27	A
	ATOM	637		E A 147	51.045	7.528	1.452	1.00 17.13 1.00 14.43	A
	ATOM	638		R A 148	52.981	6.534	0.854		A
	ATOM	639		R A 148	53.541	7.718	0.232	1.00 17.12 1.00 17.96	A
20	ATOM	640		R A 148	54.449	8.531	1.197		A
	ATOM	641		R A 148	55.605	7.760	1.537	1.00 21.51 1.00 18.83	A
	ATOM	642		R A 148	53.700	8.897	2.472		A
	ATOM	643		R A 148	54.386	7.262	-0.946	1.00 19.60 1.00 20.31	A
	ATOM	644		R A 148	54.860	6.124	-0.991	1.00 20.31	A
25	ATOM	645		E A 149	54.543	8.149	-1.916	1.00 18.94	A
	MOTA	646		E A 149	55.368	7.877	-3.073	1.00 19.16	A A
	ATOM	647		E A 149	54.748	6.801	-3.989	1.00 17.23	A
	ATOM	648		E A 149	53.389	7.144	-4.544	1.00 17.23	A
	ATOM	649	CD1 PH		53.262	7.888	-5.712	1.00 10.00	A
30	ATOM	650		E A 149	52.235	6.668	-3.927	1.00 10.30	A
	ATOM	651		E A 149	52.007	8.149	~6.267	1:00 19.26	A
	ATOM	652		E A 149	50.972	6.923	-4.470	1.00 19.17	A
	ATOM	653		E A 149	50.858	7.663	-5.642	1.00 19.17	A
	ATOM	654		E A 149	55.542	9.205	-3.774	1.00 20.85	A
35	ATOM	655	O PHI	E A 149	54.934	10.200	-3.376	1.00 19.76	A A
	MOTA	656		N A 150	56.398	9.241	-4.782	1.00 19.79	· A
	MOTA	657	CA GL	N A 150	56.636	10.481	-5.497	1.00 24.03	A
	MOTA	658	CB GL1	V A 150	57.659	11.347	-4.739	1.00 24.45	A
	MOTA	659	CG GLN	N A 150	58.986	10.645	-4.414	1.00 26.28	· A
40	ATOM	660	CD GLN	N A 150	59.988	11.558	-3.692	1.00 29.02	A
	ATOM	661	OE1 GLN	N A 150	60.693	12.353	-4.321	1.00 27.05	· A
	ATOM	662	NE2 GLN	7 A 150	60.042	11.449	-2.365	1.00 26.47	A
	ATOM	663	C GLN	A 150	57.160	10.203	-6.885	1.00 23.88	A
	ATOM	664	O GLN	I A 150	57.673	9.118	-7.158	1.00 24.79	A
45	MOTA	665		A 151	56.987	11.171	-7.774	1.00 25.88	A
	ATOM	666	CA ASP	A 151	57.527	11.047	-9.117	1.00 26.49	A
	ATOM	667		A 151	56.437	11.126 -	-10.199	1.00 24.54	A
	ATOM	668		A 151	55.544	12.336 -	-10.064	1.00 24.95	A
50	ATOM	669	OD1 ASP		56.005	13.379	-9.561	1.00 22.44	A
50	ATOM	670	OD2 ASP		54.369	12.242 -	-10.490	1.00 25.72	A
	ATOM	671		A 151	58.515	12.203	-9.220	1.00 28.63	A
	ATOM	672		A 151	58.890	12.780	-8.194	1.00 27.83	A
	ATOM	673		A 152	58.934	12.560 -	-10.426	1.00 29.21	Α
e e	ATOM	674		A 152	59.907	13.636 -	-10.562	1.00 31.88	Α
55	ATOM	675		A 152	60.325	13.792 -		1.00 33.94	A
	ATOM	676	CG ASP	A 152	61.033	12.564 -		1.00 38.88	A
	ATOM	677	OD1 ASP		61.817	11.959 -		1.00 39.67	A
	ATOM	678	OD2 ASP		60.817	12.211 -		1.00 41.57	A
	ATOM	679	C ASP	A 152	59.487	14.994 -	10.013	1.00 30.90	A

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	ATOM	680	0	ASP A	152	60.316	15.735	-9.482	1.00	31.69	Α
	ATOM	681	N	GLU A	•	58.207		-10.107		29.44	A
	ATOM	682	CA	GLU A		57.767	16.632	-9.646		28.69	A
	ATOM	683	СВ	GLU A		56.984		-10.766		32.90	A
5	ATOM	684	CG	GLU A		57.451		-12.183		40.57	A
•	ATOM	685	CD	GLU A		56.920		-12.675		45.78	A
	ATOM	686	OE1	GLU A		55.682		-12.760		48.91	A
	ATOM	687		GLU A		57.736		-12.979		48.95	A
	ATOM	688	C	GLU A		56.929	16.683	-8.372		26.43	A
10	ATOM	689	Õ	GLU A		56.947	17.688	-7.660		25.08	A
10	ATOM	690	N	LYS A		56.205	15.610	-8.069		22.39	A
	ATOM	691	CA	LYS A		55.318	15.631	-6.912		21.43	A
	ATOM	692	CB	LYS A		53.861	15.628	-7.398		20.33	A
	ATOM	693	CG	LYS A		53.505	16.716	-8.403		21.92	A
15	ATOM	694	CD	LYS A		52.211	16.375	-9.146		19.70	A
13	ATOM	695	CE	LYS A		51.775		-10.077		20.04	A
	ATOM	696	NZ	LYS A		50.631		-10.951		19.97	A
	ATOM	697	C	LYS A		55.458	14.522	-5.881		20.43	A
	ATOM	698	Ö	LYS A		55.949	13.426	-6.173		21.13	A
20	ATOM	699	N	LEU A		54.985	14.832	-4.676		19.69	A
20	ATOM	700	CA	LEU A		54.950	13.900	~3.553		19.10	A
	ATOM	701	CB	LEU A		55.362	14.588	-2.252		19.65	A
	MOTA	702	CG	LEU A		56.740	15.234	-2.129		21.20	A
	ATOM	703	CD1	LEU A		56.848	15.918	-0.770		23.42	A
25	ATOM	704	CD2	LEU A		57.816	14.174	-2.277		23.08	A
23	ATOM	704	CDZ	LEU A		53.478	13.507	-3.427		18.87	A
,	ATOM	706	o	LEU A		52.600	14.348	-3.620		18.61	A
	ATOM	707	N	TYR A		53.209	12.249	-3.020		15.02	A
	ATOM	708	CA	TYR A		51.834	11.783	-2.934		16.29	A
30	ATOM	709	CB	TYR A		51.470	10.769	-4.029		14.20	A
30	ATOM .	710	CG	TYR A		51.603	11.273	-5.449		17.29	A
	ATOM	711	CD1	TYR A		52.857	11.429	-6.045		16.46	A
	ATOM	712	CE1	TYR A		52.978	11.884	-7.360		18.68	A
•	ATOM	713	CD2	TYR A		50.474	11.588	-6.202		16.43	A
35	ATOM	714	CE2			50.583	12.048	-7.512		16.31	. A
55	ATOM	715	CZ	TYR A		51.835	12.192	-8.083		18.17	A
	ATOM	716	ОН	TYR A		51.941	12.651	-9.371		17.47	A
	ATOM	717	C	TYR A		51.657	11.108	-1.572		16.32	A
	ATOM	718	o .	TYR A		52.412	10.197	-1.235		16.27	Α
40	ATOM	719	N	PHE A		50.678	11.568	-0.792	1.00	15.47	Α
	ATOM	720	CA	PHE A		50.385	10.966	0.508		16.66	. А
•	ATOM	721	CB	PHE A		50.324	12.014	1.629		16.91	Α
	ATOM	722	CG	PHE A		51.631	12.708	1.907	1.00	18.96	A.
	ATOM	723	CD1	PHE A		52.821	12.261	1.340		20.31	A
45	ATOM	724		PHE A		51.664	13.829	2.732		21.12	A
	ATOM	725		PHE A		54.025	12.926	1.585		22.08	Α
	ATOM	726		PHE A		52.865	14.500	2.982		22.18	А
	ATOM	727	CZ	PHE A		54.045	14.045	2.405		21.27	Α
	ATOM	728	C	PHE A		49.016	10.308	0.404	1.00	16.52	А
50	ATOM	729	Ō.	PHE A		48.029	10.979	0.110	1.00	17.32	A
•	ATOM	730	N	GLY A		48.953	9.002	0.644		15.97	A
	ATOM	731	CA	GLY A		47.684	8.299	0.572		16.13	A
	ATOM	732	C	GLY A		47.000	8.383	1.920		14.94	A
	ATOM	733	Ö	GLY A		47.445	7.756			16.28	A
55	ATOM	734	N	LEU A		45.915	9.145	1.989		13.50	A
	ATOM	735	CA	LEU A		45.191	9.340	3.241		15.20	A
	ATOM	736	СВ	LEU A		45.031	10.835	3.517		14.20	A
	ATOM	737	CG	LEU A		46.270	11.726	3.385	1.00	19.00	Α
	ATOM	738		LEU A		45.847	13.188	3.477		17.12	A
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	ATOM	739	CD2	LEU	A	159		47.275	11.390	4.471	1.00	14.71	A
	ATOM	740	С			159		43.809	8.716	3.232	1.00	15.53	А
	ATOM	741	0			159		43.232	8.472	2.177	1.00	16.05	Α
	MOTA	742	N			160		43.268	8.469	4.418	1.00	15.86	Α
5	ATOM	743	CA			160		41.932	7.917	4.498	1.00	19.01	A
	ATOM	744	CB			160		41.566	7.582	5.949	1.00	22.90	A
	ATOM	745	OG			160		41.901	8.629	6.833	1.00	24.18	A
	ATOM	746	С			160		40.987	8.968	3.924	1.00	20.43	A
	ATOM	747	0	SER	A	160		41.213	10.173	4.062	1.00	19.96	A
10	ATOM	748	N			161		39.945	8.508	3.250	1.00	19.20	A
	MOTA	749	CA			161		38.975	9.406	2.644	1.00	20.37	A
	ATOM	750	CB	TYR	A	161		38.471	8.785	1.332	1.00	20.00	A
	ATOM '	751	CG			161		37.314	9.502	0.666	1.00	20.72	A
	MOTA	752	CD1	ΤΥR				37.222	10.895	0.682	1.00	18.22	A
15	ATOM	753	CE1	TYR	Α	161		36.180	11.557	0.029	1.00	22.24	Α.
	ATOM	754		TYR				36.333	8.784	-0.020	1.00	20.53	A
	MOTA	755	CE2	TYR				35.287	9.436	-0.678	1.00	24.24	A
	ATOM	756	CZ	TYR	A	161		35.218	10.822	-0.648	1.00	22.32	. A
	MOTA	757	OH	TYR				34.194	11.471	-1.298		23.03	A
20	ATOM	758	С	TYR				37.812	9.681	3.598		20.14	A
	ATOM	759	0	TYR	А	161		36.959	8.819	3.810	1.00	19.53	A
	MOTA	760	N	ALA				37.791	10.880	4.178		19.92	A
	ATOM	761	CA	ALA				36.721	11.271	5.099		21.07	A
	ATOM	762	CB	ALA				37.187	12.419	6.002		19.60	A
25	ATOM	763	С	ALA				35.542	11.712	4.238		22.07	. А
	ATOM	764	0	ALA				35.436	12.875	3.860		20.66	A
	MOTA	765	N	LYS				34.653	10.769	3.945		23.27	A
	ATOM	766	CA	LYS				33.503	11.017	3.080		27.12	A
	ATOM	767	CB	LYS			-	32.663	9.741	2.963		29.68	A
30	MOTA	768	CG	LYS				33.455	8.524	2.515		37.67	A
	ATOM	769	CD	LYS				32.556	7.310	2.321		42.24	A
	ATOM	770	CE	LYS				33.373	6.034	2.185		44.48	A
	ATOM	771	NZ	LYS				34.143	5.735	3.430		44.88	A
25	ATOM	772	С	LYS				32.581	12.186	3.411		25.78	A
35	ATOM	773	0	LYS				32.103	12.863	2.506		26.53	A A
	MOTA	774	N	ASN				32.327	12.441	4.689 5.033		24.57 23.77	A
	ATOM	775	CA	ASN				31.420 30.610	13.522 13.129	6.265		25.02	A
	ATOM	776	CB	ASN				29.537	12.101	5.932		27.54	A
40	ATOM	777 778	CG ·	ASN ASN				28.772	12.281	4.983		28.79	A
40	ATOM ATOM	779		ASN				29.475	11.024	6.704		27.13	A
	ATOM	780	C	ASN				31.999	14.931	5.169		24.43	A
	ATOM	781	0	ASN				31.306	15.856	5.589		23.98	A
	ATOM	782	N	GLY				33.262	15.097	4.795		21.56	A
45	ATOM	783	CA	GLY				33.873	16.414	4.836		24.39	A
73	ATOM	784	C	GLY				34.191	17.043	6.181		23.62	A
	ATOM	785	o	GLY				34.380	16.352	7.177		23.26	A
	ATOM	786	N	GLU				34.234	18.373	6.186		23.22	A
	ATOM	787	CA	GLU			•	34.563	19.176	7.362		24.54	A
50	ATOM	788	СВ	GLU				35.055	20.558	6.913		25.04	A
-	ATOM	789	CG	GLU				36.419	20.569	6.229		26.48	A
	ATOM	790	CD	GLU				36.699	21.889	5.517		30.02	A
	ATOM	791		GLU				36.081	22.906	5.889		29.33	A
	ATOM	792		GLU				37.544	21.916	4.596		30.48	A
55	ATOM	793	C	GLU				33.436	19.372	8.369		24.44	A
	ATOM	794	ō	GLU				32.279	19.541	8.001		22.76	A
	ATOM	795	N	LEU				33.791	19.370	9.649		22.95	Α
	ATOM	796	CA	LEU				32.813	19.581	10.707		22.26	A
	ATOM	797	CB	LEU				33.497	19.481	12.073		22.32	A

	. ATOM ATOM	798 799			A 167 A 167	32.706 31.454	19.923 19.074			22.04	A
	ATOM	800			A 167	33.597				19.66	A
	ATOM	801			A 167	32.193				21.17	A
5	ATOM	802	-		A 167	31.047		10.529 10.907		23.49	Α
	ATOM	803	-		A 168	32.960		9.948		23.56	A
	ATOM	804			A 168	32.473		9.722		24.25	A
	ATOM	805			A 168	33.560		9.066		26.64	A
	ATOM	806			A 168	33.198		8.707		25.62	A
10	ATOM	807			A 168	32.718		9.946		27.34	A
	ATOM	808			A 168	34.418		8.119		26.74	A
	ATOM	809			A 168	31.234		8.829		27.13	A
	ATOM	810	0		A 168	30.297		9.030		26.01	A A
	ATOM	811	N		A 169	31.233		7.848		26.41	A
15	ATOM	812	CA		A 169	30.106		6.934		27.70	A
	ATOM	813	СВ		A 169	30.324	21.064	5.945		30.49	A
	ATOM	814	CG		A 169	29.151	20.854	4.993		32.47	A
	ATOM	815	CD	LYS	A 169	29.407	19.728	3.998		35.98	A
	ATOM	816	CE	LYS	A 169	29.462	18.372	4.683		38.53	A
20	ATOM	817	NZ	LYS	A 169	29.622	17.263	3.702		41.00	A
	MOTA	818	С	LYS	A 169	28.801	21.985	7.682		28.12	A
	MOTA	819	0	LYS	A 169	27.785	22.608	7.371		28.08	A
	ATOM	820	N	TYR	A 170	28.826	21.094	8.668		26.53	A
	MOTA	821	CA	TYR	A 170	27.624	20.791	9.434		26.95	A
25	MOTA	822	CB	TYR	A 170	27.810	19.476	10.193		25.03	A
	ATOM	823	CG		A 170	27.898	18.300	9.251		26.65	A
	MOTA	824	CD:	LTYR	A 170	26.745	17.661	8.790		28.27	A
	ATOM	825			A 170	26.814	16.642	7.839		26.85	A
20	ATOM	826		TYR		29.127	17.884	8.742		27.83	A
30	ATOM	827		YYR		29.209	16.869	7.792		27.19	A
	ATOM	828	CZ		A 170	28.049	16.254	7.343	1.00	30.02	A
	ATOM	829	ОН		A 170	28.130	15.268	6.382		29.23	A
	ATOM	830	С		A 170	27.229	21.918	10.376		27.59	Α
35	ATOM -		0		A 170	26.045	22.122	10.642		29.25	Α
22	ATOM	832	N		A 171	28.208	22.660	10.882		28.16	Α
	ATOM	833 834	CA		A 171	27.883	23.770	11.763		29.03	Α
	ATOM	835		ILE A	A 171	. 29.151	24.435	12.337		27.51	A
	ATOM	836		ILE A		28.773 29.872	25.705	13.084		27.97	A
40	ATOM	837		ILE A			23.458	13.272		26.70	A
	ATOM	838	C		A 171	31.163 27.094	23.996	13.856		24.07	A
	ATOM	839	Ö		4 171	26.088	24.796 25.335	10.944 11.407		31.41	A
	ATOM	840	N		A 172	27.546	25.047	9.719		31.69 33.21	A
	ATOM	841	CA	ARG A		26.874	26.000	8.844		36.54	A
45	ATOM	842	CB			27.734		7.616			A
	ATOM	843	CG	ARG A		29.057	27.011	7.912		37.73 41.65	A
	ATOM	844	CD	ARG A		29.708	27.492	6.616		45.29	A A
	MOTA	845	NE	ARG P		31.037	28.070	6.812	1.00		A
	MOTA	846	CZ	ARG A	172	31.314	29.059	7.658	1.00		A
50	MOTA	847	NH1	ARG A	172	30.355	29.593	8.406	1.00		A
	ATOM	848	NH2	ARG A	172	32.553	29.526	7.748	1.00		A
	ATOM	849	С	ARG A	172	25.528	25.459	8.378	1.00		A
	ATOM	850	0		172	24.550	26.200	8.288	1.00		A
~ ~	ATOM	851	N	LYS A		25.481	24.163	8.092	1.00		A
55	ATOM	852	CA	LYS A		24.259	23.528	7.619	1.00		A
	ATOM	853	CB	LYS A		24.523	22.061	7.272	1.00		A
	ATOM	854	CG	LYS A		23.279	21.298	6.830	1.00		A
	ATOM	855	CD	LYS A		23.557	19.808	6.653	1.00		A
	ATOM	856	CE	LYS A	173	24.477	19.530	5.469	1.00	52.63	A

	ATOM	857	NZ	LYS	a a	173	23.855	19.894	4.160	1.00	54.61		71
•	ATOM	858	C			173	23.089	23.608	8.595		39.30		A
	ATOM	859	Ö			173						•	A
							21.981	23.960	8.201		39.62		Α
_	ATOM	860	N			174	23320	23.282	9.863		37.96		Α
5	ATOM	861	CA			174	22.229	23.314	10.833	1.00	37.36		Α
	ATOM	862	CB	ILE	: A	174	22.159	21.998	11.652	1.00	37.44		Α
	MOTA	863	CG2	: ILE	A	174	22.058	20.802	10.709	1.00	38.37		Α
	ATOM	864	CG1	ILE	: A	174	23.397	21.850	12.532		37.25		A
	ATOM	865	CD1			174	23.355	20.620	13.418		36.85		A
10	ATOM	866	C			174	22.259	24.492	11.801		36.71		
	ATOM	867	ō			174	21.448						A
								24.556	12.724		38.05		A
	ATOM	868	N			175	23.185	25.423	11.592		35.48		Α
•	ATOM	869	CA			175	23.265	26.585	12.462		35.29		Α
	ATOM	870	С	GLY	Α	175	24.053	26.360	13.737	1.00	35.06		Α
15	ATOM	871	0	$\operatorname{GL} Y$	Α	175	25.066	27.019	13.970	1.00	37.46		A
	ATOM	872	N	SER	A	176	23.581	25.441	14.571	1.00	33.94		Α
	ATOM	873	CA	SER	A	176	24,253	25.113	15.822		32.84		A
	ATOM	874	CB			176	23.938	26.155	16.901		33.54		A
	ATOM	875	OG			176	22.599	26.056	17.347		34.86		
20	ATOM	876	C			176	23.796						A
								23.731	16.276		32.34		A
•	ATOM	877	0			176	22.726	23.263	15.884		32.82		A
	MOTA	878	Ŋ			177	24.609	23.085	17.103	1.00	29.39		Α
	ATOM	879	CA	PHE	A	177	24.313	21.743	17.597	1.00	27.20		Α
	MOTA	880	CB	PHE	Α	177	25.621	20.989	17.865	1.00	26.39		Α
25	ATOM	881	CG	PHE	Α	177	26.372	20.585	16.622	1.00	26.18		A
	ATOM	882	CD1	PHE	Α	177	26.210	21.277	15.426		25.30		A
	ATOM	883		PHE			27.266	19.516	16.662		26.05		A
	ATOM	884		PHE			26.923	20.912	14.290		26.59		A
•	ATOM	885	CE2				27.986	19.143	15.532				
30	ATOM	886									26.06		A
50			CZ			177	27.815	19.841	14.343		25.42		A
	ATOM	887	C			177	23.500	21.752	18.884		27.00		Α
	ATOM	888	0	PHE	A	177	23.704	22.610	19.747	1.00	26.48		A
	ATOM	889	N	ASP	Α	178	22.578	20.802	19.022	1.00	26.70		A
	ATOM	890	CA	ASP	A	178	21.816	20.729	20.260	1.00	26.35		Α
35	ATOM	891	CB	ASP	Α	178	20.621	19.773	20.142	1.00	29.90		Α
	ATOM	892	CG	ASP			21.020	18.372	19.720	•	32.28		A
	ATOM	893	OD1	ASP			22.157	17.949	20.014		35.21		A
	ATOM	894		ASP			20.179	17.683	19.105		34.79		A
	ATOM	895	C	ASP			22.810	20.228	21.311		25.03		
40	ATOM	896	Ö	ASP			23.974						A
-10								19.968	20.992		21.24		A
	MOTA	897	N	GLU			22.361	20.083	22.552		23.60		Α
	ATOM	898	CA	GLU			23.247	19.644	23.619		25.18		Α
	ATOM	899	СВ	GLU			22.542	19.770	24.971	1.00	27.60		Α
	ATOM	900	CĆ	GLU	Α	179	23.324	19.176	26.130	1.00	32.58		Α
45	ATOM	901	CD	${ t GLU}$	Α	179	22.997	19.845	27.449	1.00	35.82		Α
	ATOM	902	OE1	GLU	A	179	21.825	20.224	27.645		35.95		Α
	ATOM	903	OE2	GLU	Α	179	23.912	19.984	28.291		38.19		A
	ATOM	904	·C	GLU			23.808	18.235	23.450		24.08		A
	ATOM	905	Ö	GLU			24.977	17.989	23.756		22.79	•	
50	ATOM	906	N	THR			22.983	17.316					A.
20	ATOM								22.961		23.36	*	A
		907	CA	THR			23.412	15.935	22.761		22.15		Α
	ATOM	908	CB	THR			22.224	15.054	22.320		23.77		Α
	ATOM	909		THR			21.222	15.075	23.341	1.00	26.37		Α
	MOTA	910	CG2	THR	A	180	22.670	13.616	22.088	1.00	22.66		A
55	MOTA	911	С	THR	Α	180	24.533	15.830	21.724	1.00	22.01		Α
	ATOM	912	0	THR			25.533	15.141	21.944		19.87		A
	ATOM	913	N	CYS			24.365	16.511	20.596		21.21		A
	ATOM	914	CA	CYS			25.372	16.480	19.541		22.22		A
-	ATOM	915	CB	CYS			24.800	17.065					
		213	CD	U13			23.000	11.000	18.250	1.00	24.62		A

	ATOM	916	SG .	CYS	Α	181	23.435	16.080	17.560	1.00	29.50		A
	ATOM	917	С			181	26.633	17.232	19.954	1.00	23.07		Α
	ATOM	918	0	CYS	Α	181	27.746	16.827	19.608	1.00	23.95		A
	ATOM	919	N	THR	Α	182	26.463	18.325	20.695	1.00	22.76		A
5	ATOM	920	CA	THR	Α	182	27.606	19.103	21.161		21.49		A
	ATOM	921	CB	THR	Α	182	27.167	20.346	21.978		21.37		A
	ATOM	922	OG1	THR	Α	182	26.459	21.262	21.134		22.50		A
	ATOM	923	CG2	THR	Α	182	28.379	21.046	22.565		18.36		A
	ATOM	924	С	THR	Α	182	28.454	18.215	22.071		21.48		A
10	ATOM	925	0	THR	Α	182	29.669	18.090	21.894		19.95		A
	ATOM	926	N	ARG	Α	183	27.798	17.602	23.050		18.97		A
	ATOM	927	CA	ARG	Α	183	28.468	16.723	23.996		19.39		A
	ATOM	928	СВ	ARG	Α	183	27.455	16.140	24.984		19.46		A
	ATOM	929	CG	ARG	Α	183	28.030	15.062	25.887		18.77		Α
15	MOTA	930	CD	ARG	Α	183	27.021	14.571	26.925		21.19		A
	ATOM	931	NE			183	26.605	15.642	27.824		19.46		A
	ATOM	932	CZ			183	25.496	16.362	27.679		20.45		A
	ATOM	933		ARG			24.672	16.123	26.666		19.81		A
	ATOM	934		ARG			25.224	17.338	28.539		17.11		A
20	ATOM	935	С			183	29.206	15.577	23.302		20.02		A
	ATOM	936	0	ARG			30.383	15.333	23.573		19.97		A
,	ATOM	937	N			184	28.520	14.871	22,409		19.24		A
	ATOM	938	CA	PHE	Α	184	29.144	13.746	21.722		18.04		A
	ATOM	939	СВ	PHE			28.158	13.078	20.764	1.00			. A
25	ATOM	940	CG	PHE			28.719	11.857	20.098		22.67		A
	ATOM	941	CD1	PHE	Α	184	28.717	10.630	20.754	1.00	22.97		Α
	ATOM	942	CD2				29.317	11.949	18.850		19.97		A
	MOTA	943	CE1	PHE	Α	184	29.308	9.510	20.176	1.00	23.53		Α
	ATOM	944	CE2	PHE	À	184	29.915	10.833	18.263	1.00	24.11		Α
30	ATOM	945	CZ	PHE	Α	184	29.910	9.613	18.928	1.00	22.97		Α
	ATOM	946	С	PHE	Α	184	30.403	14.127	20.941	1.00	17.99		A
	ATOM	947	0	PHE	A	184	31.461	13.531	21.130	1.00	18.89		Α
	ATOM	948	N	TYR	Α	185	30.292	15.110	20.056	1.00	15.73		Α
	ATOM	949	CA	TYR	A	185	31.443	15.519	19.265	1.00	15.72		Α
35	ATOM	950	CB	TYR	Α	185	30.992	16.413	18.111	1.00	17.33		Α
	ATOM	951	CG	TYR	Α	185	30.364	15.584	17.015	1.00	19.37		Α
	ATOM	952	CD1	TYR	Α	185	31.159	14.809	16.168	1.00	16.53		Α
	ATOM	953	CE1	TYR	Α	185	30.590	13.952	15.232	1.00	18.12		Α
	ATOM	954	CD2	TYR	Α	185	28.976	15.484	16.892	1.00	18.18	-	Α
40	MOTA	955	CE2	TYR	Α	185	28.398	14.623	15.956	1.00	18.90		Α
	MOTA	956	CZ	TYR	Α	185	29.211	13.861	15.133	1.00	18.41		Α
	ATOM	957	OH	TYR	A	185	28.650	12.995	14.218		20.48		Α
	MOTA	958	С	TYR			32.544	16.172	20.083		15.79		A
	ATOM	959	0	TYR			33.720	16.015	19.766		17.69		Α
45	ATOM	960	N	THR			32.176	16.887	21.142		15.68		A
	ATOM	961	CA	THR			33.184	17.504	21.997		16.03		Α
	ATOM	962	CB	THR			32.559	18.403	23.094		16.62		Α
	MOTA	963	OG1				31.866	19.503	22.481		14.79		A
	ATOM	964	CG2	THR			33.656	18.953	24.019		14.68		Α
50	MOTĄ	965	С	THR			33.954	16.375	22.680		15.59		Α
	MOTA	966	0	THR			35.176	16.443	22.823		13.77		Α
	ATOM	967	N	ALA			33.234	15.333	23.097		14.06		A
	ATOM	968	CA	ALA			33.869	14.196	23.757		14.74		A
	ATOM	969	CB	ALA		-	32.810	13.195	24.224		14.32		A
55	ATOM	970	С	ALA			34.875	13.509	22.821		14.41		A
	ATOM	971	0	ALA			35.972	13.136	23.247		15.61		A
	ATOM	972	N	GLU			34.516	13.340	21.549		14.01		A
	ATOM	973	CA	GLU			35.443	12.704	20.615		13.50		A
	ATOM	974	·CB	GLU	Α	T88	34.782	12.449	19.251	1.00	12.85		Α

	ATOM	975	.CG	GLU .	A 188	33.	622	11.454	19.282	1.00	12.71	A
	MOTA	976			A 188	33.	464	10.685	17.979		15.01	A
	ATOM	977		GLU .		33.	687	11.275	16.899		13.21	A
_	ATOM	978		GLU 2		33.	110	9.484	18.031		17.69	A
5	ATOM	979		GLU	A 188	36.	682	13.582	20.436		13.34	A
	MOTA	980	0		A 188	37.	803	13.085	20.408	1.00	14.69	A
	MOTA	981	N	ILE 2	A 189	36.	486	14.893	20.326		13.52	A
	ATOM	982	CA	ILE 2	A 189	37.	627	15.787	20.159		13.35	A
	MOTA	983	CB		A 189	37.	169	17.247	19.939		13.95	A
10	MOTA	984		ILE A		38.	381	18.165	19.822		12.47	A
	ATOM	985		ILE A		36.	302	17.332	18.671	1.00	13.44	A
	ATOM	986	CD1			35.	588	18.664	18.491		14.29	A
	ATOM	987	С	ILE A	189	38.	530	15.702	21.394	1.00	14.63	A
	MOTA	988	0	ILE A	189	39.	753	15.595	21.271		12.97	А
15	MOTA	989	N	VAL A	190	37.	927	15.751	22.582	1.00	14.35	Α
	MOTA	990	CA	VAL A	190	38.	684	15.655	23.832		13.22	A
	ATOM	991	CB	VAL A	190	37.	743	15.690	25.061		14.28	A
	ATOM	992		VAL A	190	38.	509	15.267	26.326		15.08	Α
	ATOM	993	CG2	VAL A	190	37.	160	17.082	25.233	1.00	12.08	A
20	MOTA	994	С	VAL F	190	39.	468	14.338	23.859	1.00	14.61	A
	ATOM	995	0	VAL A	190	40.	634	14.304	24.250		13.72	А
	ATOM	996	N	SER A	191	38.	825	13.254	23.432	1.00	15.26	A
	ATOM	_. 997	CA	SER A	191	39.	478	11.943	23.421		16.81	A
	MOTA	998	CB	SER A	191	38.	470	10.857	23.041	1.00	16.14	A
25	AŢOM	999	OG	SER A	191	39.0	018	9.569	23.238	1.00	16.94	A
	ATOM	1000	С	SER A	: 191	40.	649	11.928	22.441	1.00	16.58	А
	MOTA	1001	0	SER A	191	41.	697	11.335	22.713	1.00	13.96	A
	ATOM	1002	N	ALA A		40.4	468	12.586	21.300	1.00	15.26	A
	MOTA	1003	CA	ALA A		41.	518	12.645	20.292	1.00	14.37	A
30	ATOM	1004	CB	ALA A	. 192	40.9	989	13.296	19.016	1.00	14.43	A
	MOTA	1005	С	ALA A	192	42.6	695	13.440	20.845	1.00	16.46	A
	MOTA	1006	0	ALA A		43.8	851	13.038	20.697	1.00	17.96	A
	ATOM	1007	N	LEU A		42.4	401	14.563	21.496	1.00	15.02	A
	ATOM	1008	CA	LEU A		43.4		15.392	22.067	1.00	15.42	A
35	MOTA	1009	CB	LEU A		42.8	384	16.712	22.600	1.00	12.88	A
	MOTA	1010	CG	LEU A		42.4		17.721	21.525	1.00	15.97	A'
	ATOM	1011		LEU A		41.8	369	18.979	22.190	1.00	13.97	. A
	MOTA	1012		LEU A		43.6	542	18.088	20.655	1.00	14.58	A
40	ATOM	1013	С	LEU A		44.2		14.659	23.174		14.49	A
40	ATOM	1014	0	LEU A		45.4		14.813	23.310		16.56	A
	ATOM	1015		GLU A		43.5		13.870	23.975		13.96	A
	ATOM	1016		GLU A		44.1		13.123	25.032		14.08	A
	MOTA	1017		GLU A		43.1		12.295	25.857		14.65	A
4.5	ATOM	1018		GLU A		43.8		11.301	26.789		17.09	A
45	ATOM	1019		GLU A		42.9		10.592	27.730		19.59	Α
	ATOM	1020		GLU A		41.8		10.237	27.295		19.25	A
	ATOM	1021		GLU A		43.3		10.380	28.906		20.20	A
	ATOM	1022		GLU A		45.2		L2.199	24.386		13.57	A
50	ATOM	1023		GLU A		46.3		12,093	24.847		14.23	A
50	ATOM	1024		TYR A		44.8		L1.544	23.301		14.89	A
	ATOM	1025		TYR A		45.7		10.642	22.618		16.58	A
	ATOM	1026		TYR A		45.0		9.910	21.488		17.29	A
	ATOM	1027		TYR A		45.9		9.058	20.649		17.92	A
5.5	ATOM	1028		TYR A		46.3		7.788	21.077		17.96	A
55	ATOM	1029		TYR A		47.2		6.996	20.304		19.77	Α
	ATOM	1030		TYR A		46.4		9.524	19.428	1.00		A
	ATOM	1031		TYR A		47.2		8.744	18.650	1.00		A
	ATOM	1032		TYR A		47.6		7.481	19.094	1.00		A
	ATOM	1033	OH '	TYR A	195	48.5	υ6	6.705	18.325	1.00	21.89	A

	ATOM	1034	С	TYR A	A 195		46.917	11.419	22.035	1.00 16.98	А
	ATOM	1035	0	TYR A	195		48.081	11.047	22.203	1.00 14.61	Á
	ATOM	1036	N		1 196		46.599	12.507	21.347	1.00 16.30	A
	ATOM	1037	CA	LEU A			47.619	13.328	20.720	1.00 10.30	A
5	ATOM	1038	СВ	LEU A			46.969	14.502	19.982	1.00 18.13	
	ATOM	1039	CG	LEU A			47.834	15.203	18.935	1.00 18.59	A
	ATOM	1040		LEU A			48.222	14.206	17.841		A
	ATOM	1041		LEU A			47.060	16.375		1.00 20.94	A
	ATOM	1042	C	LEU F	_		48.592		18.338	1.00 22.98	A
10	ATOM	1042	Ö	LEU A			49.801	13.844	21.763	1.00 17.75	A
10	ATOM	1043	N	HIS F			49.001	13.644	21.649	1.00 18.33	A
	ATOM	1044						14.495	22.792	1.00 17.12	A
	ATOM		CA	HIS A			48.913	15.042	23.842	1.00 18.47	A
		1046	CB	HIS A			48.069	15.866	24.817	1.00 15.90	Α
16	ATOM	1047	CG	HIS A			47.571	17.152	24.231	1.00 19.15	A
15	ATOM	1048		HIS A			47.830	17.745	23.038	1.00 18.22	A
	ATOM	1049		HIS A			46.704	17.992	24.897	1.00 17.47	A
	ATOM	1050		HIS A			46.450	19.047	24.139	1.00 19.74	A
	ATOM	1051		HIS A			47.119	18.921	23.007	1.00 15.69	A
	ATOM	1052	С	HIS A			49.696	13.958	24.572	1.00 19.40	A
20	ATOM	1053	0	HIS A			50.823	14.192	25.021	1.00 19.42	A
	MOTA	1054	N	GLY A			49.106	12.770	24.679	1.00 18.59	A
	ATOM	1055	CA	GLY A			49.793	11.675	25.339	1.00 19.60	A
	MOTA	1056	С	GLY A			51.075	11.307	24.612	1.00 21.86	, A
	MOTA	1057	0	GLY A			51.963	10.682	25.186	1.00 23.09	A
25	MOTA	1058	N	LYS A			51.174	11.687	23.341	1.00 22.81	A.
	MOTA	1059	CA	LYS A			52.368	11.401	22.549	1.00 24.43	A
	MOTA	1060	CB	LYS A			51.990	10.905	21.154	1.00 26.00	A
	MOTA	1061	CG	LYS A	199		51.378	9.520	21.133	1.00 30.98	A
	ATOM	1062	CD	LYS A	199		51.291	9.002	19.708	100 36.85	Α
30	MOTA	1063	CE	LYS A	199		50.832	7.559	19.682	1.00 40.37	A
	MOTA	1064	NZ	LYS A	199		51.646	6.691	20.581	1.00 43.48	A
	MOTA	1065	С	LYS A	199		53.253	12.631	22.414	1.00 23.88	A
	ATOM	1066	0	LYS A	199		54.144	12.669	21.568	1.00 24.97	Ą
	ATOM	1067	N	GLY A	200		52.997	13.638	23.243	1.00 24.00	A
35	MOTA	1068	CA	GLY A	200		53.790	14.853	23.203	1.00 22.12	A
	MOTA	1069	С	GLY A	200		53.665	15.632	21.907	1.00 22.14	A
	ATOM	1070	0	GLY A	200		54.632	16.231	21.439	1.00 22.41	A
	ATOM	1071	N	ILE A	201	•	52.475	15.630	21.320	1.00 20.00	A
	ATOM	1072	CA	ILE A	201		52.252	16.355	20.080	1.00 18.93	А
40	ATOM	1073	CB	ILE A	201		51.784	15.414	18.955	1.00 19.70	A
	MOTA	1074	CG2	ILE A	201		51.414	16.226	17.716	1.00 20.12	A
	ATOM	1075	CG1	ILE A	201		52.880	14.395	18.636	1.00 20.03	A
	ATOM	1076	CD1	ILE A			52.408	13.258	17.745	1.00 22.75	A
	ATOM	1077	С	ILE A	201		51.193	17.425	20.270	1.00 19.87	A
45	ATOM	1078	0	ILE A	201		50.121	17.161	20.817	1.00 20.08	A
	MOTA	1079	N	ILE A	202		51.508	18.633	19.815	1.00 19.94	A
	MOTA	1080	CA	ILE A	202		50.601	19.772	19.891	1.00 20.45	A
	ATOM	1081	CB	ILE A	202		51.352	21.040	20.356	1.00 22.21	A
	ATOM	1082	CG2	ILE A	202		50.381	22.220	20.470	1.00 22.67	A
50	ATOM	1083	CG1	ILE A	202		52.033	20.775	21.700	1.00 24.19	Α
	ATOM	1084	CD1	ILE A	202		52.914	21.920	22.169	1.00 25.39	A
	ATOM	1085	С	ILE A	202		50.105	19.999	18.464	1.00 20.71	A
	MOTA	1086	0	ILE A	202		50.910	20.067	17.538	1.00 19.48	Α
	ATOM	1087	N	HIS A			48.795	20.108	18.270	1.00 18.65	A
55	ATOM	1088	CA	HIS A			48.280	20.319	16.919	1.00 18.02	A
	ATOM	1089	CB	HIS A			46.775	20.057	16.874	1.00 16.31	A
	ATOM	1090	CG	HIS A			46.199	20.136	15.495	1.00 18.36	A
	ATOM	1091	CD2	HIS A			46.043	21.186	14.655	1.00 16.42	A
	ATOM	1092		HIS A			45.759	19.026	14.806	1.00 19.50	A
										•	

	MOTA	1093		1 HIS			45.359	19.389	13.600	1.00 17.64	. A
	ATOM	1094	NE	2 HIS	A 203	·	45.522	20.694	13.483	1.00 20.87	. A
	ATOM	1095			A 203		48.589	21.738	16.405	1.00 18.92	A
	ATOM	1096	0	HIS	A 203		49.073	21.906	15.282	1.00 16.21	A
5	MOTA	1097	N		A 204		48.301	22.744	17.232	1.00 18.21	
	ATOM	1098	CA		A 204		48.552	24.157	16.914		Α
	ATOM	1099	СВ		A 204		49.998	24.365	16.458	1.00 19.81	A
	ATOM	1100	CG		A 204		51.024	24.137		1.00 21.61	A
	ATOM	1101	CD		A 204				17.550	1.00 23.82	A
10	ATOM	1102	NE				52.323	24.870	17.252	1.00 27.62	A
10					A 204		52,932	24.449	15.994	1.00 29.43	A
	ATOM	1103	CZ		A 204		54.125	24.861	15.572	1.00 33.10	A
	ATOM	1104	NH		A 204		54.835	25.706	16.311	1.00 32.12	A
	ATOM	1105		2 ARG			54.614	24.426	14.418	1.00 30.25	A
	ATOM	1106	C		A 204		47.624	24.830	15.905	1.00 20.03	A
15	ATOM	1,107	0	ARG .	A 204		47.711	26.038	15.698	1.00 20.88	A
	ATOM	.1108	N	ASP I	A 205		46.755	24.071	15.255	1.00 18.96	A
	MOTA	1109	CA	ASP I	A 205		45.828	24.692	14.325	1.00 17.90	A
	MOTA	1110	CB	ASP I	A 205.		46.418	24.741	12.914	1.00 18.95	A
	ATOM	1111	CG	ASP Z	A 205		45.655	25.688	12.008	1.00 20.36	A
20	ATOM	1112	OD:	L ASP			44.939	26.560	12.545	1.00 20.35	A
	ATOM	1113		2 ASP A			45.772	25.573	10.771	1.00 22.49	A
	ATOM	1114	С		A 205		44.500	23.956	14.328	1.00 19.60	A
	ATOM	1115	ō		A 205		43.876	23.751	13.287	1.00 13.00	
	ATOM	1116	N		A 206		44.063	23.569	15.521	1.00 21.53	A
25	ATOM	1117	CA		1 206		42.813	22.851	15.667		A
23	ATOM	1118	CB		1 206					1.00 19.18	A
	ATOM	1119	CG		1 206		42.693	22.295	17.087	1.00 18.94	A
	ATOM	1120					41.511	21.358	17.346	1.00 23.10	A
				LEU A			41.615	20.142	16.436	1.00 23.01	A
20	ATOM	1121		LEU A			41.504	20.933	18.808	1.00 22.97	A
30	ATOM	1122	С	LEU A			41.639	23.772	15.361	1.00 19.05	А
	ATOM	1123	0	LEU A			41.556	24.880	15.886	1.00 19.25	A
	ATOM	1124	N	LYS A			40.740	23.307	14.500	1.00 17.54	A
	ATOM	1125	CA	LYS P			39.564	24.081	14.110	1.00 18.60	A
	ATOM	1126	CB	LYS F	207		39.980	25.248	. 13.196	1.00 18.98	A
35	MOTA	1127	CG	LYS F	207		40.786	24.817	11.982	1.00 18.20	Α
	ATOM	1128	CD	LYS F	207		41.246	26.000	11.139	1.00 21.42	A
	ATOM	1129	CE	LYS F	207		42.223	25.537	10.062	1.00 23.21	A
	ATOM	1130	NZ	LYS F	207		42.561	26.604	9.084	1.00 29.61	· A
	ATOM	1131	С	LYS F	207		38.566	23.181	13.388	1.00 18.18	A
40	ATOM	1132	0	LYS A			38.921	22.100	12.915	1.00 18.11	A
	ATOM	1133	N	PRO A			37.298	23.614	13.293	1.00 20.26	. A
	ATOM	1134	CD		208.		36.713	24.833	13.882	1.00 20.20	A
	ATOM	1135	CA	PRO A			36.272	22.814	12.616	1.00 10.73	A
	ATOM	1136	CB	PRO A			35.063	23.742	12.608	1.00 19.67	
45	ATOM	1137									A
.5	ATOM		CG C	PRO A			35.231	24.509	13.891	1.00 21.81	A
		1138		PRO A			36.674	22.372	11.209	1.00 21.04	A
	ATOM	1139	0	PRO A			36.264	21.307	10.751	1.00 21.19	A
	ATOM	1140	N	GLU A			37.474	23.188	10.528	1.00 21.69	A
=-	MOTA	1141	CA	GLU A			37.928	22.872	9.170	1.00 22.64	Α
50	ATOM	1142	CB	GLU A			38.644	24.084	8.558	1.00 23.65	А
	ATOM	1143	CG	GLU A			39.253	23.825	7.185	1.00 27.24	A
	ATOM	1144	CD	GLU A	209		40.155	24.958	6.716	1.00 29.40	A
	ATOM	1145		GLU A			39.660	26.094	6.553	1.00 29.68	A
	MOTA	1146	OE2	GLU A	209		41.363	24.711	6.511	1.00 30.07	A
55	MOTA	1147	С	GLU A	209		38.879	21.668	9.159	1.00 22.28	A
	ATOM	1148	0	GLU A			38.955	20.933	8.170	1.00 21.36	A
	MOTA	1149	N	ASN A			39.600	21.490	10.263	1.00 19.90	A
	ATOM	1150	CA	ASN A			40.574	20.412	10.436	1.00 19.44	A
	ATOM	1151	СВ	ASN A			41.744	20.912	11.287	1.00 20.07	A
								-0.712		2.00 20.07	**

	ATOM	1152	CG	ASN	A 210		42.746	21.698	10.479	1.00 25,77	. А
	ATOM	1153	OD	l ASN	A 210		43.571			1.00 26.73	. A
	ATOM	1154	ND:	2 ASN	A 210		42.687	21.548		1.00 25.15	A
	MOTA	1155	С	ASN	A 210		40.005	19.151	11.078	1.00 18.63	A
5	ATOM	1156	0	ASN	A 210		40.712	18.154	11.234	1.00 18.29	A
	MOTA	1157	N	ILE	A 211		38.739		11.469	1.00 16.31	A
	ATOM	1158	CA	ILE	A 211		38.090		12.085	1.00 15.49	A
	MOTA	1159	CB	ILE	A 211		37.336	18.488	13.354	1.00 15.40	A
	ATOM	1160	CG	2 ILE	A 211		36.582	17.311	13.950	1.00 14.59	A
10	ATOM	1161	CG:	LILE	A 211		38.342		14.365	1.00 15.91	A
	ATOM	1162	CD:	LILE	A 211		37.720	19.669	15.590	1.00 15.98	A
	MOTA	1163	С	ILE	A 211		37.131		11.059	1.00 17.26	A
	MOTA	1164	0	ILE	A 211		35.995	17.947	10.926	1.00 18.16	A
	MOTA	1165	N	LEU	A 212		37.599		10.317	1.00 15.97	A
15	ATOM	1166	CA	LEU	A 212		36.784	15.875	9.274	1.00 17.08	A
	MOTA	1167	СВ	LEU	A 212		37.685	15.249	8.202	1.00 17.78	A
	ATOM	1168	CG	LEU	A 212		38.785	16.157	7.640	1.00 18.92	A
	ATOM	1169	CD1	. LEU	A 212		39.476	15.450	6.485	1.00 22.09	A
	ATOM	1170	CD2	LEU	A 212		38.188	17.482	7.166	1.00 19.91	A
20	ATOM	1171	С		A 212		35.843	14.825	9.837	1.00 18.35	A
	ATOM	1172	0		A 212	•	35.957	14.433	11.002	1.00 19.39	A
	MOTA	1173	N		A 213		34.915	14.368	9.000	1.00 17.84	A
	ATOM	1174	CA		A 213		33.942	13.362	9.403	1.00 19:94	A
	ATOM	1175	CB		A 213		32.556	14.004	9.487	1.00 20.84	A
25	MOTA	1176	CG		A. 213		32.396	15.059	10.583	1.00 20.31	. A
	ATOM	1177	CD1		A 213		31,124	15.837	10.367	1.00 22.75	A
	MOTA	1178	CD2	LEU	A 213		32.379	14.378	11.940	1.00 23.93	A
	ATOM	1179	С		A 213		33.914	12.187	8.426	1.00 20.98	A
	MOTA	1180	0		A 213		33.743	12.379	7.218	1.00 19.55	A
30	ATOM	1181	N		A 214		34.088	10.970	8.935	1.00 20.44	A
	ATOM	1182	CA		A 214		34.055	9.814	8.049	1.00 23.77	A
	ATOM	1183	CB		A 214		34.745	8.596	8.674	1.00 25.30	· A
	ATOM	1184	CG		A 214		34.077	8.127	9.948	1.00 32.04	A
	ATOM	1185	OD1		A 214		32.908	8.422	10.206	1.00 34.43	A
35	ATOM	1186			A 214		34.818	7.369	10.752	1.00 33.85	A
	ATOM	1187	С		A 214		32.618	9.466	7.693	1.00 24.07	A
	ATOM	1188	0		A 214		31.672	10.113	8.150	1.00 19.94	A
	ATOM	1189	N		A 215		32.459	8.433	6.879	1.00 25.77	A
	ATOM	1190	CA		A 215		31.138	8.003	6.445	1.00 28.69	A
40	ATOM	1191	СВ		A 215		31.275	6.796	5.513	1.00 31.98	A
	ATOM	1192	CG		A 215		29.970	6.334	4.896	1.00 40.22	Ā
	ATOM	1193	CD		A 215		30.182	5.312	3.795	1.00 44.27	A
	ATOM	1194	OE1		A 215		30.817	4.268	4.065	1.00 46.46	A
	ATOM	1195	OE2		A 215		29.716	5.556	2.660	1.00 46.13	A
45	MOTA	1196	С		A 215		30.188	7.673	7.601	1.00 28.41	A
	ATOM	1197	O		A 215		28.971	7.769	7.447	1.00 28.52	A
	ATOM	1198	N		A 216		30.737	7.287	8.752	1.00 26.77	A
	ATOM	1199	CA		A 216		29.914	6.953	9.917	1.00 27.28	A
	ATOM	1200	CB		A 216		30.538	5.795	10.696	1.00 27.20	A
50	ATOM	1201	CG		A 216		30.390	4.466	9.979	1.00 37.61	A
	ATOM	1202			A 216		29.274	4.170	9.499	1.00 37.01	A
	ATOM	1203			A 216		31.382	3.710	9.902	1.00 41.84	A
	ATOM	1204	C		A 216		29.697	8.135	10.862	1.00 41.34	A
	ATOM	1205	Õ		A 216		29.136	7.984	11.950	1.00 25.73	A
55	ATOM	1206	N .		A 217		30.156	9.306	10.441	1.00 23.73	A
. =	ATOM	1207	CA		A 217		30.135	10.527	11.218	1.00 23.02	A
	ATOM	1208	CB		A 217		28.537	10.789	11.517	1.00 21.83	A
	ATOM	1209	CG		A 217		27.742	11.186	10.274	1.00 23.24	A
	ATOM	1210	SD		A 217		28.464	12.616	9.430	1.00 22.96	A A
							-0.101	72.010	2.130	1.00 2/.3/	n

	ATOM	1211	CE	MET	Α	217		27.679	13.974	10.332	1.00 26.68	A
	ATOM	1212	С	MET	A	217		30.844	10.618	12.502	1.00 21.51	
	ATOM	1213	ō			217		30.474	11.323	13.440	1.00 21.51	
	ATOM	1214	N			218		31.957	9.892		•	A
5			CA							12.544	1.00 20.10	A
,	ATOM	1215				218		32.873	9.964	13.678	1.00 19.86	A
	ATOM	1216	CB			218		33.482	8.594	13.977	1.00 20.21	A
	ATOM	1217	CG			218		32.551	7.667	14.698	1.00 22.40	A
	ATOM	1218		HIS				31.910	6.547	14.287	1.00 21.27	A
	ATOM	1219		HIS				32.177	7.863	16.011	1.00 19.59	A
10	ATOM	1220		HIS				31.348	6.902	16.379	1.00 21.88	Α
	ATOM	1221	NE2	HIS	Α	218		31.168	6.091	15.351	1.00 22.08	A
	ATOM	1222	С	HIS	Α	218		33.947	10.921	13.172	1.00 19.10	A
	ATOM	1223	0	HIS	Α	218		34.170	11.004	11.965	1.00 20.31	A
•	ATOM	1224	N			219		34.617	11.638	14.067	1.00 17.21	A.
15	ATOM	1225	CA			219		35.628	12.586	13.618	1.00 17.21	A
10.	ATOM	1226	CB			219		35.987	13.614	14.716	1.00 15.20	
	ATOM	1227		ILE				34.722	14.305			A
				ILE						15.221	1.00 14.58	A
	ATOM	1228						36.734	12.919	15.864	1.00 14.46	A
00	ATOM	1229		ILE				37.279	13.885	16.911	1.00 13.74	A
20	MOTA	1230	С			219		36.929		13.161	1.00 16.21	A
	ATOM	1231	0			219		37.238	10.799	13.500	1.00 15.88	A
	MOTA	1232	N	GLN				37.677	12.711	12.378	1.00 15.62	A
	MOTA	1233	CA	GLN	Α	220		38.980	12.316	11.876	1.00 17.84	A
	MOTA	1234	CB	GLN	Α	220		38.872	11.595	10.525	1.00 20.00	A
25	ATOM	1235	CG	GLN	Α	220		38.463	10.129	10.659	1.00 26.97	A
	ATOM	1236	CD	GLN	Α	220		38.648	9.343	9.372	1.00 29.95	Α
	ATOM	1237	OE1	GLN	A	220		37.968	9.590	8.373	1.00 33.12	Α
	MOTA	1238	NE2	GLN	Α	220		39.578	8.393	9.389	1.00 30.47	A
	ATOM	1239	С	GLN	Α	220		39.757	13.610	11.735	1.00 17.00	A
30	MOTA	1240	0	GLN				39.609	14.339	10.751	1.00 18.27	A
	ATOM	1241	N	ILE				40.566	13.906	12.746	1.00 14.34	A
	ATOM	1242	CA	ILE				41.361	15.120	12.753	1.00 14.46	A
	ATOM	1243	CB	ILE				41.867	15.416	14.175	1.00 12.30	, A
	ATOM	1244		ILE				42.764	16.656	14.167	1.00 12.30	A
35	ATOM	1245		ILE				40.660	15.613	15.102	1.00 13.92	A
55	ATOM	1245		ILE				41.003	15.901	16.543	1.00 15.06	A
			CDI					•				A
	ATOM	1247		ILE				42.536	14.996	11.783	1.00 15.44	
	ATOM	1248	0	ILE				43.106	13.915	11.613	1.00 13.93	A
40	ATOM	1249	N	THR				42.877	16.101	11.127	1.00 15.36	A
40	MOTA	1250	CA	THR				43.980	16.098	10.174	1.00 17.52	A
	ATOM	1251	CB	THR				43.470	15.836	8.750	1.00 19.92	A
	ATOM	1252		THR			•	44.587	15.637	7.875	1.00 18.78	A
	AŢOM	1253	CG2	THR				42.630	17.018	8.257	1.00 18.16	A
	ATOM	1254	С	THR				44.735	17.428	10.192	1.00 19.60	A
45	ATOM	1255	0	THR	Α	222		44.509	18.257	11.084	1.00 18.59	. A
	ATOM	1256	N	ASP	А	223		45.630	17.610	9.216	1.00 18.69	А
	ATOM	1257	CA	ASP	Α	223		46.440	18.825	9.069	1.00 20.12	A
	MOTA	1258	СВ	ASP	Α	223		45.532	20.065	9.108	1.00 23.51	Α
	ATOM	1259	CG	ASP	Α	223		46.248	21.335	8.670	1.00 27.09	Α
50	ATOM	1260		ASP				47.283	21.227	7.975	1.00 26.28	A
	ATOM	1261		ASP				45.765	22.438	9.009	1.00 26.15	Α
	ATOM	1262	C	ASP			•	47.516	18.913	10.150	1.00 21.73	A
	ATOM	1263	0	ASP				47.439	19.751	11.055	1.00 22.76	A
	ATOM	1263	N	PHE				48.535	18.063	10.027	1.00 22.76	A
55		1265						49.611			1.00 20.75	A
,,	MOTA		CA	PHE					17.988	11.009	1.00 20.11	
	ATOM	1266	CB	PHE				49.805	16.527	11.424		. A
	ATOM	1267	CG	PHE				48.682	15.991	12.263	1.00 21.41	· A
	ATOM	1268		PHE				48.598	16.312	13.614	1.00 23.05	A
	ATOM	1269	CD2	PHE	A	224		47.681	15.212	11.693	1.00 22.27	A

	ATOM,	1270	CE1	. PHE F	224		47.528	15.868	14.389	1.00	23.30	A
	ATOM	1271	CE2	PHE A	224		46.606	14.763	12.457			A
	ATOM	1272	cz	PHE A			46.530	15.093	13.807	1.00	22.02	· A
	ATOM	1273	С	PHE A	224		50.957	18.583	10.619			A
5	ATOM	1274	0	PHE A	224		51.905	18.547	11.407	1.00 2		A
	ATOM	1275	N	GLY A	225		51.049	19.125	9.412	1.00 2		A
	ATOM	1276	CA	GLY A	225		52.301	19.713	8.981	1.00 2		A
	MOTA	1277	С	GLY A			52.742	20.822	9.920	1.00 2		A
	MOTA	1278	0	GLY A		•	53.939	21.041	10.122	1.00 2		A
10	ATOM	1279	N	THR A			51.779	21.524	10.508	1.00 2		A
	MOTA	1280	CA	THR A	226		52.106	22.613	11.416	1.00 2		A
•	ATOM	1281	CB	THR A			51.199	23.829	11.160	1.00 2		A
	ATOM	1282	OG1				49.831	23.410	11.113	1.00 2		A
	ATOM	1283		THR A			51.571	24.490	9.834	1.00 2		A
15	ATOM	1284	C	THR A			52.046	22.233	12.894	1.00 2		A
	ATOM	1285	Ö	THR A			52.019	23.100	13.768	1.00 2		A
	ATOM	1286	N	ALA A			52.013	20.935	13.173	1.00 2		A
	ATOM	1287	CA	ALA A			52.004	20.475	14.550	1.00 2		A
	ATOM	1288	CB	ALA A			51.659	18.993	14.607	1.00 2		A
20	ATOM	1289	CD	ALA A			53.384	20.715	15.149	1.00 2		A A
20	MOTA	1290	Ö	ALA A			54.331	21.047	14.435			
	ATOM	1291	N	LYS A								A
	ATOM	1292	CA	LYS A			53.491	20.558	16.461	1.00 2		A
		1292					54.760		17.149	1.00 3		A
25	MOTA		CB	LYS A			54.699	21.974	18.054	1.00 3		A
23	ATOM	1294	CG	LYS A			56.007	22.294	18.765		1.23	· A
	ATOM	1295	CD				57.082	22.725	17.768	1.00 4		A
	ATOM	1296	CE	LYS A			58.401	23.056	18.462	1.00 4		A
	ATOM	1297	NZ	LYS A			59.459	23.425	17.480	1.00 5		A
20	ATOM	1298	C	LYS A			55.019	19.504	17.985	1.00 3		A
30	ATOM	1299	0	LYS A			54.190	19.129	18.815	1.00 3		A.
	ATOM	1300	N	VAL A			56.159	18.860	17.756	1.00 3		Α
	ATOM	1301	CA	VAL A			56.516	17.661	18.501	1.00 3		A
•	ATOM	1302	CB	VAL A			57.248	16.646	17.609	1.00 3		A
25	ATOM	1303		VAL A			57.619	15.419	18.415	1.00 3		A
35	ATOM	1304		VAL A			56.370	16.264	16.436	1.00 3		A
	ATOM	1305	С	VAL A			57.420	18.035	19.668	1.00 3		A
	ATOM	1306	0	VAL A			58.581	18.392	19.474	1.00 3		A
	ATOM	1307	N	LEU A			56.877	17.948	20.878	1.00 4		A
40	ATOM	1308	CA	LEU A			57.615	18.289	22.088		6.10	A
40	MOTA	1309	CB	LEU A			56.654	18.417	23.270	1.00 4		A
	ATOM	1310	CG		230		55.627	19.545	23.207	1.00 4		A
	ATOM	1311		LEU A			54.673	19.430	24.383	1.00 4		A
	ATOM	1312		LEU A			56.340	20.885	23.214	1.00 4		A
45	ATOM	. 1313	С	LEU A			58.695	17.279	22.440	1.00 5		A
43	ATOM	1314	0	LEU A			58.603	16.104	22.089	1.00 5		A
	ATOM	1315	N	SER A			59.717	17.756	23.145	1.00 5		A
	MOTA	1316	CA	SER A			60.824	16.914	23.583	1.00 6		A
	ATOM	1317	CB	SER A			62.077	17.200	22.750	1.00 6		A
50	ATOM	1318	OG	SER A			62.444	18.568	22.823	1.00 6		A
50	ATOM	1319	С	SER A			61.124	17.126	25.071	1.00 6		A
	ATOM	1320	0	SER A			61.392	16.164	25.794	1.00 6		A
	ATOM	1321	N	PRO A			61.081	18.387	25.549	1.00 6		A
	ATOM	1322	CD	PRO A			60.854	19.651	24.823	1.00 6		A
	ATOM	1323	CA	PRO A			61.358	18.655	26.966	1.00 6		A
55	ATOM	1324	CB	PRO A			61.109	20.158	27.086	1.00 6		A
	ATOM	1325	CG	PRO A			61.505	20.666	25.737	1.00 6		A
	ATOM	1326	C	PRO A			60.460	17.846	27.899	1.00 6		A
	ATOM	1327	0	PRO A			59.335	17.494	27.541	1.00 6		A
	ATOM	1328	N	ALA A	237		57.424	23.198	27.637	1.00 8	0.06	A

						_				
	AŢOM	1329	9 CF	ALA A 237		56.783	23,047	26.335	1.00 79.29	74
	ATOM	1330) CE	•		55.275	•			A
	ATOM			ALA A 237		57.092				A
	ATOM	1332		ALA A 237						A
5	ATOM	1333		ALA A 238		56.250				A
•	ATOM	1334				58.297		–		A
						58.683			1.00 78.50	A
	ATOM	1335				60.186		23.728	1.00 78.50	A
	ATOM	1336		ALA A 238		57.920	25.327	22.673	1.00 78.15	A
	ATOM	1337		ALA A 238		57.243	24.341	22.375		A
10	ATOM	1338	N	ALA A 239		58.027	26.393		1.00 77.28	A
	ATOM	1339	CA	ALA A 239		57.338		20.603		A
	ATOM	1340	CB			55.849			1.00 76.61	
	ATOM	1341	С	ALA A 239		57.766		19.793	1.00 75.38	A
	ATOM	1342	0	ALA A 239		58.955	27.955	19.700		A
15	ATOM	1343		ASN A 240		56.781			1.00 75.89	A
	ATOM	1344		ASN A 240			28.357	19.214	1.00 73.95	A
	ATOM	1345				56.967	29.553	18.389	1.00 71.07	A
	ATOM	1346		ASN A 240		58.151	30.400	18.874	1.00 71.47	Α
				ASN A 240		59.459	30.055	18.174	1.00 72.06	Α
20	ATOM	1347	OD.	1 ASN A 240		59.575	30.149	16.943	1.00 72.03	Α
20	ATOM	1348		2 ASN A 240		60.470	29.665	18.964	1.00 71.91	A
	MOTA	1349	С	ASN A 240		57.188	29.178	16.928	1.00 69.41	A
	MOTA	1350	0	ASN A 240		57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	N	ALA A 241		57.055	30.165	16.038	1.00 66.62	A
	ATOM	1352	CA	ALA A 241		57.246	30.013	14.585	1.00 63.94	A
25	ATOM	1353	С	ALA A 241		55.952	30.080	13.772	1.00 60.63	
	ATOM	1354	0	ALA A 241		55.840	30.880	12.845	1.00 61.29	A
	`ATOM	1355	СВ	ALA A 241		57.979	28.704	14.246		A
	ATOM	1356	N	PHE A 242		54.984	29.236	14.113	1.00 65.23	A
	ATOM	1357	CA	PHE A 242		53.712	29.196		1.00 56.72	A
30	ATOM	1358	СВ	PHÈ A 242		53.419	27.767	13.394	1.00 52.53	A
	ATOM	1359	CG	PHE A 242		52.040		12.923	1.00 49.14	A
	ATOM	1360		PHE A 242			27.590	12.354	1.00 47.38	A
	ATOM	1361	CD3	PHE A 242		51.731	28.067	11.085	1.00 47.69	Α
	ATOM	1362		PHE A 242		51.038	26.975	13.102	1.00 45.45	A
35	ATOM	1363	CET	PHE A 242		50.445	27.937	10.565	1.00 46.75	A
	ATOM	1364				49.751	26.840	12.594	1.00 45.41	A
	ATOM		CZ	PHE A 242	•	49.453	27.323	11.322	1.00 46.55	Α
	-	1365	С	PHE A 242		52.534	29.688	14.229	1.00 50.08	Α
	ATOM	1366	0	PHE A 242		52.502	29.505	15.444	1.00 49.86	A
40	ATOM	1367	N	VAL A 243		51.566	30.305	13.557	1.00 47.67	Α
40	ATOM	1368	CA	VAL A 243		50.355	30.809	14.200	1.00 46.21	A
	ATOM	1369	CB	VAL A 243		50.340	32.352	14.258	1.00 47.36	Α
	MOTA	1370		VAL A 243		49.012	32.844	14.825	1.00 47.54	A
	ATOM	1371	CG2	VAL A 243		51.497	32.842	15.109	1.00 48.50	A
	MOTA	1372	С	VAL A 243		49.150	30.342	13.389	1.00 44.12	A
45	ATOM	1373	0	VAL A 243		48.956	30.765	12.247	1.00 44.46	A
	ATOM	1374	N	GLY A 244		48.348	29.467	13.985	1.00 40.48	
	ATOM	1375	CA	GLY A 244		47.176	28.941	13.306	1.00 37.65	A
	ATOM	1376	С	GLY A 244		46.101	29.960	12.964	1.00 37.03	A
	ATOM	1377	0	GLY A 244		46.313	31.168			A
50	ATOM	1378	N	THR A 245		44.936	29.463	13.065	1.00 35.92	A
	ATOM	1379	CA	THR A 245				12.560	1.00 33.30	A
	ATOM	1380	CB	THR A 245		43.813	30.312	12.184	1.00 30.20	A
	ATOM	1381				42.593	29.450	11.829	1.00 32.00	A
	ATOM			THR A 245		42.952	28.573	10.755	1.00 32.81	A
55		1382		THR A 245		41.419	30.319	11.390	1.00 28.34	Α
55	ATOM	1383	C	THR A 245		43.476	31.296	13.296	1.00 27.96	A
	ATOM	1384	0	THR A 245		43.212	30.907	14.434	1.00 25.46	A
	ATOM	1385		ALA A 246		43.486	32.576	12.938	1.00 25.22	A
	ATOM	1386		ALA A 246		43.247	33.675	13.867	1.00 23.27	A
	ATOM	1387	CB	ALA A 246		42.956	34.955	13.082	1.00 22.94	A

	MOTA	1388	С	ALA	Α	246	42.178	33.475	14.934	1 00	21.27	A
	ATOM	1389	0		•	246	42.431	33.705	16.114		20.93	· A
	MOTA	1390	N			247	40.988	33.047	14.536		19.67	
	ATOM	1391	CA			247	39.911	32.886	15.504			A
5	ATOM	1392	CB			247	38.608				20.17	A
,	ATOM	1393						32.535	14.779		21.89	A
			CG			247	38.522	33.076	13.355		26.18	A
	ATOM	1394	CD			247	37.220	33.794	13.064		27.30	· A
	ATOM	1395		L GLN			36.172	33.447	13.605		30.13	Α
10	ATOM	1396		GLW			37.278	34.792	12.189	1.00	28.70	A
10	ATOM	1397	С			247	40.181	31.849	16.595		19.43	А
	ATOM	1398	0			247	39.546	31.883	17.648		18.93	A
	ATOM	1399	N			248	41.132	30.948	16.359	1.00	18.60	A
	ATOM	1400	· CA	TYR	Α	248	41.441	29.896	17.329	1.00	19.20	A
	MOTA	1401	CB	TYR	Α	248	41.333	28.529	16.642	1.00	17.53	A
15	MOTA	1402	CG	TYR	Α	248	40.013	28.362	15.927	1.00	19.32	Ά
	ATOM	1403	· CDI	TYR	Α	248	38.859	28.010	16.625		17.69	A
	ATOM	1404	CE1	TYR	Α	248	37.617	27.976	15.990		18.18	A
	ATOM	1405		TYR			39.897	28.664	14.569		16.87	A
	ATOM	1406		YYR			38.665	28.635	13.924		19.17	A
20	ATOM	1407	CZ			248	37.527	28.295	14.643		19.46	A
	ATOM	1408	ОН			248	36.299	28.311	14.023		18.98	
	ATOM	1409	C			248	42.810	30.039	17.993		20.42	A
	ATOM	1410	ō			248	43.208	29.191	18.792		19.19	A
	ATOM	1411	N			249	43.523	31.114	17.673		20.20	
25	ATOM	1412	CA			249	44.841	31.343	18.251		20.20	A
23	ATOM	1413	CB			249	45.542	32.532	17.570			A
	ATOM	1414		VAL.							21.18	A
	ATOM	1415		VAL			46.821 45.862	32.896	18.317		22.45	A
	ATOM	1415	C					32.170	16.139		24.01	A
30	ATOM					249	44.764	31.606	19.750		21.52	A
30		1417	0	VAL			43.915	32.368	20.216		22.72	A
	ATOM	1418	N .			250	45.654	30.965	20.503		20.70	A
	ATOM	1419	CA			250	45.697	31.133	21.951		21.65	A
	ATOM	1420	CB	SER			46.370	29.919	22.613		22.02	A
2.5	MOTA	1421	OG	SER			47.692	29.725	22.132		22.12	Α
35	MOTA	1422	С	SER			46.476	32.402	22.280		22.13	A
	ATOM	1423	0	SER			47.332	32.828	21.511		22.77	A
	ATOM	1424	N	PRO			46.180	33.029	23.425		22.23	A
	ATOM	1425	CD	PRO			45.163	32.684	24.433	1.00	22.97	A
	ATOM	1426	CA	PRO			46.893	34.254	23.800	1.00	22.52	A
40	ATOM	1427	CB	PRO			46.233	34.650	25.127	1.00	23.06	Α
	ATOM	1428	CG	PRO			45.726	33.329	25.676	1.00	22.55	A
	ATOM	1429	С	PRO	Α	251	48.414	34.115	23.907	1.00	22.15	A
	MOTA	1430	0	PRO	Α	251	49.143	35.047	23.563	1.00	22.62	A
	ATOM	1431	N	GLU	Α	252	48.901	32.966	24.367	1.00	20.69	A
45	MOTA	1432	CA	GLU	Α	252	50.347	32.772	24.500	1.00	21.40	Α
	ATOM	1433	CB	GLU	Α	252	50.673	31.382	25.071		20.59	А
	ATOM	1434	CG	GLU	A	252	49.993	30.232	24.352		21.91	A
	ATOM	1435	CD	GLU			48.691	29.822	25.014		21.51	A
	ATOM	1436	OE1	GLU	Α	252	47.989	30.707	25.550		21.46	A
50	ATOM	1437		GLU			48.367	28.613	24.993		20.23	A
	ATOM	1438	С	GLU			51.071	32.970	23.167		22.99	A
	ATOM	1439	ō	GLU			52.191	33.480	23.136		23.17	A
	ATOM	1440	N	LEU			50.441	32.576	22.064		23.17	A
	ATOM	1441	CA	LEU			51.068	32.753	20.758		25.62	A
55	ATOM	1442	CB	LEU			50.277	32.733	19.669		26.75	
	ATOM	1443	CG	LEU			50.743	30.620				A
	ATOM	1444		LEU			50.743		19.296		31.87	A N
	ATOM	1444						29.651	20.422		31.81	A
				LEU			50.044	30.179	18.015		31.86	A
	ATOM	1446	С	LEU	M.	253	51.201	34.228	20.371	1.00	26.94	A

	ATOM	1447	0	LEC	JA	253	52.107	34.601	19.626	1.00 2	7 09	A
	ATOM	1448	N	LEC	JA	254	50.297	35.059	20.877			A
	ATOM	1449	CA	LEU	J A	254	50.297	36.485	20.564			A
	ATOM	1450	CB	LEC	A	254	48.858	37.006	20.564	1.00 25		A
5	ATOM	1451	CG	LEU	A	254	47.882	36.290	19.621	1.00 24		A
	ATOM	1452	CD	1 LEU	I A	254	46.459	36.724	19.932	1.00 23		A
	ATOM	1453	CD	2 LEU	A	254	48.236	36.597	18.177	1.00 24		A
	ATOM	1454	C.			254	51.134	37.314	21.537	1.00 29		
	ATOM	1455	ō			254	51.633	38.383	21.187	1.00 30		A A
10	ATOM	1456	N			255	51.292	36.821	22.758	1.00 32		
	ATOM	1457	CA			255	52.056	37.547	23.759	1.00 32		A
	ATOM	1458	CB			255	51.368	37.478	25.127			A
	ATOM	1459		1 THR			51.188	36.106	25.127	1.00 34		A
	ATOM	1460		2 THR			50.013	38.166		1.00 35		A
15	ATOM	1461	C C			255	53.477	37.035	25.077	1.00 33		A
	ATOM	1462	Ö			255	54.430	37.033	23.910	1.00 40		A
	ATOM	1463	N			256	53.617		23.772	1.00 43		A
	ATOM	1464	CA			256	54.932	35.747	24.189	1.00 44		A
	ATOM	1465	CB			256		35.144	24.382	1.00 49		A
20	ATOM	1466	CG			256	54.866	34.143	25.534	1.00 51		A
20	ATOM	1467	CD			256	54.514	34.786	26.862	1.00 56		A
	ATOM	1468		L GLU			54.053	33.780	27.893	1.00 58		A.
	ATOM	1469		GLU			54.766	32.776	28.107	1.00 62		A
							52.979	33.996	28.494	1.00 60		A
25	ATOM ATOM	1470	С			256	55.475	34.456	23.137	1.00 50		A
23	ATOM	1471	0			256	56.616	33.995	23.127	1.00 50		A
	ATOM	1472 1473	N CA	LYS		257	54.658	34.389	22.090	1.00 51		A
	ATOM	1474	CB	LYS			55.064 56.244	33.746	20.845	1.00 51		A
	ATOM	1475	CG	LYS			56.558	34.502 34.125	20.227	1.00 53		A
30	ATOM	1476	CD	LYS			57.709	34.125	18.790 18.253	1.00 55		A
50	ATOM	1477	CE	LYS			57.709	34.694	16.777	1.00 57		A.
	ATOM	1478	NZ	LYS			58.290	33.268		1.00 58		A
	ATOM	1479	C	LYS			55.467	32.302	16.515	1.00 60		A
	ATOM	1480	Ö	LYS			56.432	31.790	21.138 20.577	1.00 50 1.00 52		A
35	ATOM	1481	N	ŞER			54.721	31.654	22.027	1.00 32		A A
-	ATOM	1482	CA	SER			54.999	30.273	22.402	1.00 46		A
	ATOM	1483	СВ	SER			55.590	30.229	23.812	1.00 48		A
•	ATOM	1484	OG	SER			54.741	30.892	24.734	1.00 48		A
	ATOM	1485	C	SER			53.735	29.415	22.342	1.00 33		A
40	ATOM	1486	Ö	SER			52.617	29.932	22.417	1.00 44		A
	ATOM	1487	N	ALA			53.917	28.105	22.204	1.00 38		A
	ATOM	1488	CA	ALA			52.793	27.180	22.127	1.00 34		· A
	ATOM	1489	CB	ALA			52.551	26.779	20.684	1.00 34		A
	ATOM.	1490	C	ALA			53.042	25.940	22.977	1.00 34		A
45	ATOM	1491	ō	ALA			54.172	25.459	23.086	1.00 32		
	ATOM	1492	N	CYS			51.975	25.428	23.579	1.00 31		A A
	ATOM	1493	CA	CYS			52.056	24.244	24.425	1.00 26		Α.
	ATOM	1494	CB	CYS			52.030	24.654	25.892	1.00 26		A
	ATOM	1495	SG	CYS			50.846	25.739	26.469	1.00 20.		A A
50	ATOM	1496	C	CYS			50.786	23.435	24.224	1.00 32		A
-	ATOM	1497	ŏ	CYS			49.892	23.856				
	ATOM	1498	N	LYS			50.706	22.277	23.495 24.868	1.00 22.		A n
	ATOM	1499	CA	LYS			49.526	21.434		1.00 20.		A
	ATOM	1500	CB	LYS			49.526	20.243	24.744 25.696			A
55	ATOM	1501	CG	LYS			50.716	19.253		1.00 23.		A
"	ATOM	1501	CD	LYS			50.716		25.347	1.00 27.		A
	ATOM	1502	CE	LYS			51.922	18.117 17.203	26.350	1.00 29.		A
	ATOM	1504	NZ	LYS			51.922	16.121	26.134 27.153	1.00 32.		A n
	ATOM	1504	C	LYS						1.00 33.		A
	ATON	1000	C	ПІЭ	Α.	COT	48.268	22.229	25.062	1.00 19.	20	Α

	ATOM	1506	5 0	LYS A	261	47	.253	22.092	24.387	1 1 00	18.08		*
	ATOM	1507	7 N	SER A			.358	23.068					A
	ATOM	1508					.235	23.883			16.92		Α
	ATOM	.1509									18.13		Α
5	ATOM	1510					. 644	24.698	27.770		18.27		A
,							.517	25.258	28.421	1.00	22.53		A
	ATOM	1511		SER A			.736	24.811	25.424	1.00	16.77		Α
•	ATOM	1512		SER A			. 591	25.254	25.450	1.00	15.69		Α
	MOTA	1513		SER A 2	263		. 595	25.118	24.456		16.44		A
	MOTA	1514	CA	SER A 2	263	47.	175	25.970	23.347		16.89		A
10	ATOM	1515	CB	SER A 2	263	48.	340	26.228	22.382		18.49		A
	ATOM	1516	OG	SER A 2	263	49.	402	26.909	23.031		22.10		
	ATOM	1517	С	SER A 2			040	25.257	22.612		17.79		A
	ATOM	1518	0	SER A 2			099	25.898	22.148				A
	ATOM	1519		ASP A 2			119	23.928			17.57		A
15	ATOM	1520		ASP A 2					22.517		16.30		A
	ATOM	1521	CB	ASP A 2			069	23.166	21.836		16.72		Α
	ATOM	1521					483	21.704	21.620	•	15.92		Α
			CG	ASP A 2			544	21.539	20.548		17.93		·A
	ATOM	1523		1 ASP A 2			642	22.412	19.661	1.00	16.78		Α
	MOTA	1524		2 ASP A 2		47.	265	20.515	20.579	1.00	16.64		Α
20	MOTA	1525	С	ASP A 2		43.	773	23.194	22.646		17.67		A
	MOTA	1526	0	ASP A 2		42.	681	23.197	22.076		18.27		A
	ATOM	1527	N	LEU A 2	265	43.	898	23.205	23.974		15.49		A
	MOTA	1528	CA	LEU A 2	265		730	23.232	24.849		14.75		A
	ATOM	1529	CB	LEU A 2	65	43.	147	23.038	26.313		11.38		A
25	MOTA	1530	CG	LEU A 2	65	43.		21.641	26.621		14.04		
	ATOM	1531	CD	L LEU A 2		44.		21.579	28.052		13.96		A
	ATOM	1532		LEU A 2		42.		20.603	26.416				A
	ATOM	1533	C	LEU A 2		41.		24.557			11.62		A
	ATOM	1534	ō	LEU A 2		40.			24.675		15.13		A
30	ATOM	1535	N	TRP A 2				24.620	24.785		16.75		А
50	ATOM	1536	CA	TRP A 2		42.		25.622	24.405		16.08		A
	ATOM	1537				42.		26.918	24.184		16.96		Α
	ATOM		CB	TRP A 2		43.		28.015	24.023		17.28		Α
		1538	CG	TRP A 2		42.		29.326	23.521	1.00	20.54		Α
25	ATOM	1539	CD2			42.3		30.490	24.301	1.00	20.07		Α
35	ATOM	1540	CE2			41.		31.459	23.417	1.00	20.46		Α
	ATOM	1541	CE3			42.4	435	30.810	25.660	1.00	20.68	•	Α
	ATOM	1542		TRP A 2		42.2	270	29.631	22.231	1.00	19.53		Α
	ATOM	1543		TRP A 2		41.7	769	30.908	22.163		19.61		Α
	ATOM	1544		TRP A 2		41.3	372	32.727	23.850		20.90		A
40	ATOM	1545	CZ3	TRP A 2	66	42.0	026	32.073	26.091		19.45		A
	ATOM	1546		TRP A 26		41.5	501	33.015	25.185		20.71		A
	ATOM	1547	С	TRP A 26		41.2		26.795	22.913		17.22		A
	MOTA	1548	0	TRP A 26		40.1		27.240	22.863		18.03		
	ATOM	1549	N	ALA A 26		41.8		26.181	21.886		17.50		A
45	ATOM	1550	CA			41.1		~-					Α
	ATOM	1551	CB	ALA A 26				25.990	20.626		16.16		A
	ATOM	1552	C	ALA A 26		42.0		25.290	19.621		14.28		Α
	ATOM	1553				39.9		25.159	20.891		16.28		A
	ATOM	1554	0	ALA A 26		38.8		25.436	20.346		16.46		Α
50			N	LEU A 26		40.0		24.144	21.739		16.57		A
50	ATOM	1555	CA.	LEU A 26		38.8		23.299	22.084	1.00	17.03		Α
	ATOM	1556	CB	LEU A 26		39.2		22.260	23.139	1.00	15.35		Α
	ATOM	1557	CG	LEU A 26		38.1		21.429	23.754	1.00			Α
	ATOM	1558		LEU A 26		37.5		20.578	22.678	1.00	16.17		Α
	ATOM	1559	CD2	LEU A 26		38.7	18	20.537	24.881	1.00			
55	MOTA	1560	С	LEU A 26	8	37.7	66	24.179	22.628	1.00			A
	ATOM	1561	0	LEU A 26		36.6			22.247	1.00			A
	ATOM	1562	N	GLY A 26	9	38.1			23.520	1.00			A
	ATOM	1563	CA	GLY A 26		37.1			24.092	1.00			A
	ATOM	1564	С	GLY A 26		36.4			23.031	1.00			A A
						20.1		_ 3.000		1.00	A 4 . J4	•	~

	ATOM			GLY	A 269		35.193	3 27.014	4 23.11	1 1 0	0 14.76	. ,
	ATOM	1566	6 N	CYS	A 270		37.146				0 13.86	
	ATOM	1567	7 CA		A 270		36.539				0 16.80	
	ATOM	1568	3 СВ		A 270		37.61					
5	ATOM	1569	9 SG		A 270		38.751				0 15.97	
	ATOM				A 270		35.598				0 20.48	
	ATOM				A 270		34.516				0 17.50	
	ATOM	1572			A 271						0 18.38	
	ATOM	1573			A 271		36.022				0 16.99	
10	ATOM	1574					35.221				0 16.66	
10	ATOM	1575			A 271		36.038				0 16.53	A
		1576		1775	A 271		35.155				0 16.34	A
	ATOM				A 271		37.222			1.0	0 15.59	A
	ATOM	1577			A 271		38.239	23.018	17.690	1.0	0 14.88	А
1.5	ATOM	1578			A 271		33.920	24.626	19.809	1.00	16.74	
15	ATOM	1579			A 271		32.865	24.576	19.179		17.12	A
	ATOM	1580		ILE .	A 272		33.990	24.357			16.13	A
	ATOM	1581			A 272		32.785	24.021			18.30	A
	ATOM	1582		ILE :	A 272		33.097				17.77	A
	ATOM	1583	CG2	ILE 2	A 272		31.796				17.96	
20	ATOM	1584			A 272		33.877	22.437			19.55	A
	ATOM	1585			A 272		34.446	22.217				A
	ATOM	1586			A 272		31.824	25.207			18.64	A
	ATOM	1587	ō		A 272		30.624	25.207	21.776		19.51	A
	ATOM	1588	N		A 273		32.362		21.554		20.44	A
25	ATOM	1589	CA		A 273	-		26.409	21.947		18.52	A
	ATOM	1590	CB		A 273		31.553	27.615	21.881		20.48	A
	ATOM	1591	CG				32.418	28.847	22.162		18.98	A
	ATOM	1592		TIK	A 273		31.663	30.161	22.125		20.26	A
				TYR A			31.229	30.709	20.916		20.67	Α
30	ATOM	1593		TYR A			30.536	31.917	20.880	1.00	20.98	A
30	ATOM	1594		TYR A			31.383	30.857	23.302	1.00	19.82	A
	ATOM	1595		TYR F			30.691	32.062	23.280		20.62	A
	ATOM	1596	CZ	TYR A	273		30.271	32.587	22.067		21.15	A
	ATOM	1597	ОН	TYR A			29.588	33.776	22.049		21.86	A
	MOTA	1598		TYR A		•	30.902	27.730	20.507		21.54	A
35	ATOM	1599	0	TYR A	273		29.719	28.049	20.401		22.80	. A
	ATOM	1600	N	GLN A	274		31.676	27.454	19.461		21.05	A
	ATOM	1601	CA	GLN A	274		31.176	27.538	18.095		21.48	A
	MOTA	1602		GLN A			32.323	27.341	17.097		21.41	A
	MOTA	1603	CG	GLN A	274		31.934	27.596	15.645		23.15	
40	ATOM	1604		GLN A			33.131	27.588	14.706		24.80	A
	ATOM	1605		GLN A			34.276	27.446	15.139			A
	ATOM	1606		GLN A			32.870	27.750	13.139		22.51	A
	ATOM	1607		GLN A			30.076	26.517			22.96	A
	ATOM	1608		GLN A			29.123	26.806	17.828		21.51	A
45	ATOM	1609		LEU A			30.207		17.108		20.50	A
	ATOM	1610		LEU A				25.324	18.403		21.44	A
	ATOM	1611					29.196	24.282	18.208		20.95	A
	ATOM	1612		LEU A			29.645	22.958	18.846		19.11	Α
	ATOM			LEU A			30.775	22.182	18.159	1.00	21.43	A
50	ATOM	1613		LEU À			31.118	20.936	18.963		17.64	A
50		1614		LEU A			30.342	21.795	16.754	1.00	20.34	A.
	ATOM	1615		LEU A			27.860	24.697	18.815	1.00	21.32	А
	ATOM	1616		LEU A			26.802	24.461	18.229	1.00	19.75	A
	ATOM	1617		/AL A			27.921	25.322	19.987		19.10	A
	ATOM	1618		AL A			26.724	25.750	20.702		22.47	A
55	ATOM	1619		AL A			27.011	25.882	22.217		20.87	A
	MOTA	1620	CG1 V				25.742	26.291	22.957		19.68	A
	ATOM	1621	CG2 V				27.550	24.558	22.766		19.43	A
	MOTA	1622		'AL A			26.127	27.075	20.211		23.89	
	ATOM	1623		'AL A			24.910	27.199	20.070		24.90	A
				•	•				20.070	1.00	~ ~ • • • • •	A

										•	
	ATOM	1624	N	ALA A	277		26.983	28.062	19.965	1.00 24.56	A
	MOTA	1625	CA	ALA A	277		26.533	29.374	19.518	1.00 24.72	A
	MOTA	1626	CB	ALA A	277		27.504	30.444	19.999	1.00 24.36	A
	ATOM	1627	С	ALA A			26.378	29.458	18.005	1.00 25.76	A
5	ATOM	1628	0	ALA A	277		25.577	30.242	17.502	1.00 26.39	A
	MOTA	1629	N	GLY A	278		27.142	28.651	17.280	1.00 25.13	A
	_ ATOM	1630	CA	GLY A			27.062	28.673	15.834	1.00 25.58	A
	MOTA	1631	С	GLY A 2	278		28.163	29.524	15.231	1.00 26.50	A
	ATOM	1632	0	GLY A 2			28.374	29.510	14.015	1.00 28.17	A
10	ATOM	1633	N	LEU A 2			28.866	30.262	16.086	1.00 24.44	A
	ATOM	1634	CA	LEU A 2			29.962	31.130	15.656	1.00 25.21	A
	ATOM	1635	CB	LEU A 2	279		29.468	32.575	15.500	1.00 25.78	A
	MOTA	1636	CG	LEU A 2			28.364	32.899	14.490	1.00 28.17	A
	ATOM	1637		L LEU A 2			27.922	34.344	14.684	1.00 26.60	A
15	MOTA	1638		2 LEU A 2	279		28.862	32.670	13.071	1.00 26.52	A
	MOTA	1639	С	LEU A 2			31.093	31.116	16.687	1.00 23.47	· A
	MOTA	1640	0	LEU A 2			30.848	30.994	17.882	1.00 24.44	A
	ATOM	1641	N	PRO A 2			32.349	31.239	16.236	1.00 23.35	A
	ATOM	1642	CD	PRO A 2			32.831	31.404	14.855	1.00 22.26	A
20	ATOM	1643	CA	PRO A 2			33.464	31.239	17.189	1.00 23.81	A
	ATOM	1644	CB	PRO A 2			34.692	31.293	16.282	1.00 23.24	A
	MOTA	1645	CG	PRO A 2			34.189	32.020	15.073	1.00 24.89	Α
	MOTA	1646	С	PRO A 2			33.353	32.444	18.137	1.00 22.69	A
0.5	ATOM	1647	0	PRO A 2			32.750	33.457	17.788	1.00 22.11	A
25	ATOM	1648	N	PRO A 2			33.939	32.344	19.345	1.00 23.06	A
	ATOM	1649	CD	PRO A 2			34.810	31.223	19.734	1.00 21.37	A
	ATOM	1650	CA	PRO A 2			33.935	33.375	20.395	1.00 23.67	A
	ATOM	1651	CB	PRO A 2		-	34.781	32.751	21.509	1.00 24.89	A
20	ATOM	1652	CG	PRO A 2			34.749	31.287	21.219	1.00 25.24	. А
30	ATOM	1653	C	PRO A 2			34.481	34.752	20.017	1.00 23.75	A
	ATOM	1654	0	PRO A 2			33.869	35.781	20.317	1.00 21.02	A
	ATOM	1655	N	PHE A 2			35.644	34.763	19.379	1.00 22.17	A
	ATOM ATOM	1656	CA	PHE A 2			36.293	36.007	18.998	1.00 23.16	A
35	ATOM	1657 1658	CB	PHE A 2			37.765	35.943	19.406	1.00 21.01	A
55	ATOM	1659	CG CD1	PHE A 2 PHE A 2			37.975	35.482	20.822	1.00 22.66	A
	ATOM	1660		PHE A 2			37.806	36.361	21.888	1.00 20.06	A
	ATOM	1661		PHE A 2			38.291	34.151 35.921	21.093	1.00 20.72	A
	ATOM	1662		PHE A 2			37.947 38.433	33.702	23.206	1.00 22.66 1.00 20.97	A
40	ATOM	1663	CZ	PHE A 2			38.261	34.590	22.405	1.00 20.97	A
	ATOM	1664	C	PHE A 2			36.169	36.263	17.503	1.00 19.38	A
	ATOM	1665	Ö	PHE A 2			36.802	35.585	16.694	1.00 24.39	A A
	ATOM	1666	N	ARG A 2			35.355	37.248	17.142	1.00 24.99	Ā
	ATOM	1667	CA	ARG A 2			35.141	37.594	15.741	1.00 26.33	A
45	ATOM	1668	СВ	ARG A 2			33.721	37.209	15.316	1.00 28.91	Ā
	ATOM	1669	CG	ARG A 2			33.293	35.808	15.724	1.00 30.27	A
	ATOM	1670	CD	ARG A 2			31.904	35.493	15.188	1.00 33.36	A
	ATOM	1671	NE	ARG A 2			30.890	36.392	15.733	1.00 33.30	A
	MOTA	1672	CZ	ARG A 2			30.372	36.287	16.952	1.00 34.79	A
50	ATOM	1673		ARG A 2			30.767	35.317	17.768	1.00 35.77	A
	ATOM	1674		ARG A 2			29.458	37.156	17.359	1.00 36.12	A
	ATOM	1675	С	ARG A 2			35,328	39.096	15.544	1.00 26.47	A
	ATOM	1676	0	ARG A 2			35.029	39.888	16.438	1.00 26.28	A
	ATOM	1677	N	ALA A 2			35.818	39.486	14.373	1.00 26.70	A
55	ATOM	1678	CA	ALA A 28			36.033	40.899	14.079	1.00 27.84	A
	ATOM	1679	CB	ALA A 28			37.188	41.442	14.914	1.00 26.24	A
	ATOM	1680	С	ALA A 28			36.327	41.077	12.602	1.00 28.35	A
	ATOM	1681	0	ALA A 28			36.560	40.101	11.891	1.00 29.91	A
	ATOM	1682	N	GLY A 28			36.332	42.329	12.153	1.00 29.29	A

	ATOM	1683	CA	GLY	A 285	5	36.5 <i>7</i> 7	42.631	10.753	1.00 29.52	A
	ATOM	1684	С	GLY	A 285	5	37.893	42.156	10.168	1.00 20.32	Ä
	ATOM	1685	0	GLY	A 285	5	37.974	41.862	8.976	1.00 30.60	A
	ATOM	1686	N	ASN	A 286	5	38.939	42.097	10.983	1.00 28.49	A
5	ATOM	1687	CA		A 286		40.231	41.644	10.489	1.00 26.71	A
	ATOM	1688	СВ		A 286		41.050	42.825	9.945	1.00 26.11	A
	MOTA	1689	CG	ASN	A 286	;	41.310	43.900	10.990	1.00 27.83	A
	ATOM	1690	OD1	ASN			41.877	43.631	12.049	1.00 27.84	A
	ATOM	1691		2 ASN			40.908	45.131	10.685	1.00 27.04	A
10	ATOM	1692	С		A 286		40.997	40.924	11.584	1.00 26.03	A
	ATOM	1693	0	ASN	A 286	;	40.540	40.851	12.723	1.00 25.66	A
	ATOM	1694	N		A 287		42.162	40.391	11.239	1.00 24.81	A
	MOTA	1695	CA		A 287		42.965	39.662	12.206	1.00 27.59	A
	MOTA	1696	СВ		A 287		44.145	38.985	11.510	1.00 30.17	A
15	ATOM	1697	CG		A 287		43.776	37.632	10.931	1.00 38.21	A
	ATOM	1698	CD		A 287		44.900	36.998	10.140	1.00 41.86	A
	ATOM	1699		GLU			46.061	37.036	10.608	1.00 43.08	A
	ATOM	1700		GLU			44.612	36.449	9.052	1.00 45.22	A
	ATOM	1701	c		A 287		43.459	40.485	13.383	1.00 45.22	A
20	ATOM	1702	ō		A 287		43.382	40.030	14.521	1.00 26.41	A
	ATOM	1703	N		A 288		43.966	41.685	13.122	1.00 23.04	A
	ATOM	1704	CA		A 288		44.460	42.528	14.205	1.00 23.04	A
	ATOM	1705	СВ		A 288		44.867	43.913	13.691	1.00 21.07	A
	ATOM	1706	CG		A 288		45.275	44.858	14.805	1.00 21.07	A
25	ATOM	1707		TYR			46.533	44.762	15.405	1.00 21.23	A
	ATOM	1708	CE1		A 288		46.891	45.588	16.475	1.00 20.43	A
	ATOM	1709		TYR			44.380	45.809	15.302	1.00 22.32	A
~	ATOM	1710	CE2		A 288		44.725	46.637	16.373	1.00 23.28	A
	ATOM	1711	CZ		A 288		45.981	46.518	16.953	1.00 22.96	· A
30	ATOM	1712	OH		A 288		46.316	47.313	18.024	1.00 23.18	A
	ATOM	1713	C		A 288		43.402	42.698	15.288	1.00 21.38	A
	ATOM	1714	Ō		A 288		43.710	42.616	16.473	1.00 22.09	A
	ATOM	1715	N		A 289		42.159	42.939	14.874	1.00 21.88	A
	ATOM	1716	CA		A 289		41.055	43.130	15.811	1.00 21.98	A
35	ATOM	1717	СВ		A 289		39.821	43.673	15.078	1.00 22.90	A
	ATOM	1718	CG		A 289		39.896	45.130	14.601	1.00 26.52	A
	ATOM '	1719	CD1		A 289		38.706	45.436	13.696	1.00 26.55	A
	ATOM	1720		LEU :			39.914	46.071	15.807	1.00 23.13	A
	ATOM	1721	С		A 289		40.686	41.849	16.560	1.00 21.24	A
40	ATOM	1722	0		A 289	-	40.256	41.897	17.715	1.00 20.72	A
	ATOM	1723	N		A 290		40.843	40.708	15.900	1.00 19.62	A
	ATOM	1724	CA		A 290		40.538	39.433	16.533	1.00 18.54	A
	ATOM	1725	СВ	ILE A	A 290		40.560	38.281	15.509	1.00 18.52	A
	ATOM	1726	CG2	ILE A			40.503	36.934	16.234	1.00 17.63	A
45	ATOM	1727		ILE A			39.378	38.429	14.545	1.00 18.88	A
	ATOM	1728		ILE 2			39.421	37.483	13.357	1.00 19.81	A
	ATOM	1729	С		A 290		41.578	39.167	17.618	1.00 19.09	A
	MOTA	1730	0	ILE A			41.236	38.788	18.737	1.00 18.20	A
	ATOM	1731	N	PHE A			42.849	39.376	17.286	1.00 18.76	A
50	ATOM	1732	CA	PHE A			43.925	39.156	18.247	1.00 20.75	A
	ATOM	1733	CB	PHE A			45.286	39.434	17.606	1.00 20.71	. A
	MOTA	1734	CG	PHE A			45.644	38.480	16.503	1.00 22.92	A
	ATOM	1735		PHE A			45.065	37.214	16.443	1.00 22.98	A
	ATOM	1736		PHE A			46.588	38.830	15.543	1.00 22.91	A
55	ATOM	1737		PHE A			45.423	36.310	15.440	1.00 24.51	A
	ATOM	1738		PHE A			46.954	37.931	14.535	1.00 25.54	A
	ATOM	1739	CZ	PHE A			46.370	36.670	14.485	1.00 23.29	A
	ATOM	1740	C	PHE A		•	43.739	40.061	19.451	1.00 21.72	A
	ATOM	1741	Ō	PHE A			43.992	39.671	20.593	1.00 22.32	A
					-		-				

	ATOM	1742	N	GLN A	292		43.284	41.275	19.178	1.00 23.27	70
	MOTA	1743	CA		292	•	43.055	42.264	20.216	1.00 23.27	
	ATOM	1744	CB	GLN A			42.574	43.559			A
	ATOM	1745	CG	GLN F			42.577	44.773	19.562	1.00 25.77	A
5	ATOM	1746	CD						20.447	1.00 28.45	A
,				GLN A			42.469	46.057	19.638	1.00 29.83	Α
	ATOM	1747		1 GLN A			41.520	46.244	18.872	1.00 27.16	A
	MOTA	1748	NE:				43.449	46.944	19.799	1.00 27.61	A
	ATOM	1749	С	GLN A	292		42.018	41.733	21.204	1.00 22.97	Α
	ATOM	1750	0	GLN A	292		42.200	41.832	22.415	1.00 21.64	A
10	ATOM	1751	N	LYS A	293		40.937	41.154	20.687	1.00 21.82	A
	ATOM	1752	CA	LYS A			39.895	40.612	21.558	1.00 22.18	A
	ATOM	1753	СВ	LYS A			38.664	40.223	20.740		
	ATOM	1754	CG	LYS A			37.919	41.407		1.00 22.69	A
	ATOM	1755	, CD	LYS A					20.153	1.00 25.78	A
15							36.651	40.961	19.429	1.00 27.88	Α
15	ATOM	1756	CE	LYS A			35.857	42.161	18.926	1.00 30.85	A
	ATOM	1757	NZ	LYS A			34.612	41.750	18.214	1.00 32.98	Α
	ATOM	1758	С	LYS A			40.398	39.398	22.343	1.00 21.20	A
	MOTA	1759	0	LYS A	293		40.041	39.204	23.509	1.00 22.01	А
	ATOM	1760	N	ILE A	294		41.226	38.583	21.702	1.00 19.91	A
20	ATOM	1761	CA	ILE A	294		41.774	37.394	22.347	1.00 20.28	A
	ATOM	1762	CB	ILE A	294		42.631	36.575	21.349	1.00 18.98	A
	ATOM	1763		ILE A		•	43.481	35.550	22.098	1.00 17.70	A
	ATOM	1764		ILE A			41.716	35.897	20.318		
	ATOM	1765		. ILE A			42.467		19.178	1.00 17.93	A
25								35.237		1.00 16.21	A
23	ATOM	1766	С	ILE A			42.618	37.727	23.587	1.00 21.94	A
	ATOM	1767	0	ILE A			42.366	37.199	24.673	1.00 20.86	A
	MOTA	1768	N	ILE A			43.610	38.600	23.439	1.00 21.88	A
	ATOM	1769	CA	ILE A	295		44.461	38.934	24.582	1.00 24.25	Α
	ATOM	1770	CB	ILE A	295		45.668	39.805	24.175	1.00 23.93	A
30	ATOM	1771	CG2	ILE A	295		46.514	39.066	23.140	1.00 24.61	A
	ATOM	1772	CG1	ILE A	295	•	45.189	41.151	23.637	1.00 24.58	A
	ATOM	1773	CD1	ILE A	295		46.317	42.149	23.433	1.00 26.69	A
	ATOM	1774	С	ILE A			43.720	39.636	25.717	1.00 24.80	A
	ATOM	1775	ō	ILE A			44.214	39.687	26.842	1.00 24.76	A
35	ATOM	1776	N	LYS A			42.539	40.173	25.425	1.00 25.33	A
55		1777									
	ATOM		CA	LYS A			41.743	40.853	26.444	1.00 26.80	A
	ATOM	1778	CB	LYS A			41.178	42.170	25.894	1.00 27.39	Α
	ATOM	1779	CG	LYS A			42.240	43.141	25,413	1.00 31.79	A
	MOTA	1780	CD	LYS A			41.634	44.410	24.826	1.00 35.56	A
40	ATOM	1781	CE	LYS A	296		41.009	45.283	25.900	1.00 39.29	A
	ATOM	1782	NZ	LYS A	296		40.564	46.603	25.357	1.00 41.72	A
	MOTA	1783	С	LYS A	296		40.593	39.958	26.893	1.00 25.50	A
	MOTA	1784	0	LYS A	296		39.770	40.361	27.713	1.00 24.02	Α
	ATOM	1785	N	LEU A	297		40.550	38.742	26.349	1.00 25.67	A
45	ATOM	1786	CA	LEU A	297		39.500	37.777			A
	ATOM	1787	СВ	LEU A			39.632	37.285	28.111	1.00 24.80	A
	ATOM	1788	CG	LEU A			38.766	36.068	28.460	1.00 26.43	A
	ATOM	1789		LEU A							
							39.238	34.852	27.646	1.00 26.70	A
50	ATOM	1790		LEU A			38.856	35.777	29.951	1.00 24.84	A
50	ATOM	1791	C	LEU A			38.151	38.459	26.467	1.00 25.11	A
	MOTA	1792	0	LEU A			37.261	38.378	27.309	1.00 25.28	A
	ATOM	1793	N	GLU A			38.007	39.127	25.331	1.00 24.98	A
	MOTA	1794	CA	GLU A			36.786	39.847	25.023	1.00 25.31	A
	MOTA	1795	CB	GLU A	298		37.143	41.139	24.291	1.00 27.13	A
55	ATOM	1796	CG	GLU A			35.991	42.092	24.108	1.00 31.28	A
	MOTA	1797	CD	GLU A			36.419	43.362	23.410	1.00 34.40	A
	ATOM	1798		GLU A			37.348	44.027	23.918	1.00 35.90	A
	ATOM	1799		GLU A			35.832	43.693	22.359	1.00 36.16	A
	ATOM	1800	C	GLU A			35.766	39.057	24.207	1.00 30.10	
		1000	•	JLV A	0		55.700	33.037	24.201	1.00 23.13	A

•											
	MOTA	1801	. 0	GLU	A 298		35.832	39.017	22.979	1.00 24.35	'n
	ATOM	1802	N S		A 299	٠	34.825				A A
	ATOM	1803	CA	TYR	A 299		33.760				A
	ATOM	1804	CB	TYR	A 299		34.264				A
5	ATOM	1805	CG	TYR	A 299		34.348				
	ATOM	1806	CD	1. TYR			35.336				A
	ATOM	1807		1 TYR			35.389				A
	ATOM	1808		2 TYR			33.410			1.00 19.30	A
	ATOM	1809		2 TYR			33.456			1.00 19.41	A A
10	ATOM	1810			A 299		34.449			1.00 19.41	A
	ATOM	1811	ОН		A 299		34.511			1.00 18.77	A
٠	MOTA	1812	С		A 299		32.699		25.331	1.00 25.20	
	ATOM	1813	0		A 299		32.942		26.506	1.00 25.20	A A
	ATOM	1814	N		A 300		31.522		24.927	1.00 26.46	A
15	ATOM	1815	CA		A 300		30.467	36.710	25.891	1.00 20.94	
	ATOM	1816	СВ		A 300		29.665	37.981	26.179	1.00 35.86	. A A
	ATOM	1817	CG		A 300		29.228	38.687	24.923	1.00 33.88	
	ATOM	1818	OD:	1 ASP			28.450	38.088	24.149	1.00 45.98	A A
	MOTA	1819		2 ASP			29.666	39.840	24.707	1.00 45.69	
20	ATOM	1820	С		A 300	•	29.564	35.608	25.363	1.00 43.69	A A
	MOTA	1821	0		A 300		29.590	35.299	24.172	1.00 29.20	
	MOTA	1822	N		A 301		28.778	35.011	26.253	1.00 28.84	A A
	ATOM	1823	CA	PHE Z			27.884	33.924	25.871	1.00 28.98	A
	ATOM	1824	CB		A 301		27.818	32.854	26.968	1.00 30.48	A
25	MOTA	1825	CG	PHE A			29.147	32.279	27.356	1.00 29.17	A
	MOTA	1826	CDI	L PHE A			29.978	32.949	28.245	1.00 23.23	A
	ATOM	1827		PHE A			29.560	31.050	26.845	1.00 27.31	A
	ATOM	1828		PHE A			31.205	32.403	28.625	1.00 27.83	A
	ATOM	1829		PHE A			30.781	30.498	27.217	1.00 28.05	A
30	ATOM	1830	CZ	PHE A			31.605	31.175	28.110	1.00 28.27	. A
	ATOM	1831	С	PHE A			26.459	34.384	25.619	1.00 28.27	· A
	ATOM	1832	0	PHE A			25.946	35.261	26.317	1.00 32.20	A
	MOTA	1833	N	PRO P			25.798	33.804	24.607	1.00 32.30	A
	ATOM	1834	CD	PRO F	302		26.313	32.943	23.529	1.00 34.04	A
,35	ATOM	1835	CA	PRO P	302		24.415	34.199	24.341	1.00 35.24	A
	ATOM	1836	CB	PRO P			24.144	33.608	22.959	1.00 33.24	A
	ATOM	1837	CG	PRO P	302		25.041	32.413	22.921	1.00 35.48	Ā
	ATOM	1838	С	PRO A	302		23.567	33.561	25.444	1.00 37.39	A
	MOTA	1839	0	PRO A	302		23.935	32.518	25.986	1.00 38.49	A
40	MOTA	1840	N	ALA A			22.447	34.188	25.783	1.00 39.36	A
	ATOM	1841	CA	ALA A	303		21.572	33.692	26.843	1.00 40.65	A
	ATOM	1842	CB	ALA A	303		20.280	34.506	26.862	1.00 41.66	A
	ATOM	1843	С	ALA A	303		21.238	32.197	26.814	1.00 41.25	A
	MOTA	1844	0	ALA A	. 303		21.253	31.537	27.854	1.00 43.16	A
45	ATOM	1845	N	ALA A	304		20.945	31.665	25.631	1.00 41.04	A
	ATOM	1846	CA	ALA A			20.569	30.258	25.480	1.00 40.66	A
	ATOM	1847	CB	ALA A	304		20.121	30.004	24.040	1.00 41.36	A
	ATOM	1848	С	ALA A	304		21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	0	ALA A			21.298	28.156	26.395	1.00 40.61	A
50	MOTA	1850	N	PHE A	305		22.891	29.543	25.617	1.00 36.21	A
	MOTA	1851	CA	PHE A	305 .		24.022	28.662	25.909	1.00 32.08	A
	ATOM	1852	CB	PHE A	305		25.259	29.519	26.187	1.00 29.46	A
	ATOM	1853	CG	PHE A	305		26.536	28.917	25.690	1.00 28.15	A
	ATOM	1854	CD1	PHE A	305		27.146	27.875	26.377	1.00 26.20	A
55	ATOM	1855		PHE A			27.127	29.386	24.521	1.00 27.05	A
	ATOM	1856	CE1	PHE A	305		28.330	27.308	25.908	1.00 26.92	A
	MOTA	1857		PHE A			28.312	28.826	24.042	1.00 26.62	A
	ATOM	1858	CZ	PHE A			28.914	27.786	24.737	1.00 26.61	A
	ATOM	1859	C	PHE A			23.811	27.664	27.057	1.00 30.09	A
		•									**

	ATOM	1860	0	PHE	A 305	23.51	8 28.051	28.187	1.00 31.51	π.
	ATOM	1861	N		A 306					. A
	ATOM	1862			A 306			27.769		
	ATOM	1863	СВ		A 306					A
5	ATOM	1864	CG		A 306			27.170		A
,								25.815	1.00 27.24	A
	ATOM	1865	CD.	1 PHE	A. 306			25.622	1.00 28.40	Α
	ATOM	1866	CDZ	PHE 2	A 306	24.35	23.386	24.728	1.00 27.84	Α
	ATOM	1867		L PHE 2		21.60	L 23.603	24.365	1.00 28.05	Α
	ATOM	1868	CE	PHE 2		23.792	23.155	23.465	1.00 28.31	A
10	ATOM	1869	CZ	PHE A	4 306	22.419	23.263	23.283	1.00 28.00	A
	ATOM	1870	С	PHE 2	A 306	24.71		28.961	1.00 26.23	A
	ATOM	1871	0		306	25.92		28.811	1.00 25.59	, A
	ATOM	1872	N		A 307	24.125		30.163	1.00 26.67	
	ATOM	1873	CD		A 307	22.685		30.430	•	A
15	ATOM	1874	CA		A 307				1.00 27.95	A
13						24.842		31.405	1.00 26.59	A
	ATOM	1875	CB	PRO A		23.795		32.481	1.00 26.14	A
	ATOM	1876	CG	PRO Z		22.531		31.803	1.00 27.86	· A
	ATOM	1877	C	PRO A		26.145	25.355	31.659	1.00 25.58	Α
	ATOM	1878	0	PRO A	307	27.189	25.964	31.900	1.00 22.65	A
20	ATOM	1879	N	LYS A	308	26.085	24.031	31.620	1.00 24.46	A
	ATOM	1880	CA	LYS A	308	27.274	23.232	31.867	1.00 23.91	A
	ATOM	1881	CB	LYS A	308	26.887		32.024	1.00 23.25	A
	ATOM	1882	CG	LYS A		26.062		33.285	1.00 28.49	A
	ATOM	1883	CD	LYS A		25.618		33.466	1.00 30.17	A
25	ATOM	1884	CE	LYS F		24.760	•	34.722	1.00 33.12	
23	ATOM	1885	NZ	LYS A		24.122				A
	ATOM	1886	C	LYS F				34.860	1.00 34.13	A
						28.314		30.769	1.00 22.84	, A
	MOTA	1887	0	LYS A		29.514		31.042	1.00 22.46	A
20	ATOM	1888	N	ALA P		27.861		29.534	1.00 21.59	A
30	ATOM	1889	CA	ALA P		28.792		28.432	1.00 20.02	A
	ATOM	1890	CB	ALA A		28.056	23.856	27.106	1.00 18.80	A
	ATOM	1891	С	ALA A	309	29.481	25.191	28.662	1.00 21.41	A
	MOTA	1892	0	ALA A	309	30.680	25.335	28.427	1.00 21.39	Α
	MOTA	1893	N	ARG A	310	28.717	26.179	29.121	1.00 21.39	A
35	ATOM	1894	CA	ARG A	310	29.290		29.388	1.00 22.02	. A
	ATOM	1895	CB	ARG A		28.213		29.854	1.00 22.39	A
	ATOM	1896	CG	ARG A		28.806		30.436	1.00 25.30	A
	ATOM	1897	CD	ARG A		27.780		30.664	1.00 28.33	A
	ATOM	1898	NE	ARG A		28.420		31.230	1.00 20.33	A
40	ATOM	1899	CZ	ARG A		27.901	33.263	31.203	1.00 30.10	
	ATOM	1900		ARG A		26.719				A
	ATOM	1901					33.477	30.634	1.00 31.19	A
				ARG A		28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	C	ARG A		30.376	27.388	30.458	1.00 21.65	A
4.5	ATOM	1903	0	ARG A		31.464	27.949	30.311	1.00 20.36	A
45	ATOM	1904	N	ASP A		30.074	26.677	31.541	1.00 19.57	A
•	ATOM	1905	CA	ASP A		31.043	26.512	32.615	1.00 20.18	Α
	ATOM	1906	CB	ASP A	311	30.460	25.649	33.739	1.00 20.39	A
•	ATOM	1907	CG	ASP A	311	31.439	25.446	34.881	1.00 23.35	A
	ATOM	1908	OD1	ASP A	311	32.158	24.428	34.885	1.00 24.91	Α
50	ATOM	1909		ASP A		31.500	26.312	35.776	1.00 26.96	A
	ATOM	1910	С	ASP A		32.322	25.877	32.073	1.00 19.73	A
	ATOM	1911	Ō	ASP A		33.422	26.289	32.439	1.00 19.30	A
	ATOM	1912	N	LEU A		32.179	24.891	31.188	1.00 15.30	A
	ATOM	1913	CA	LEU A		33.349	24.031	30.611		
55	ATOM	1914		LEU A					1.00 16.66	A
33			CB			32.927	23.035	29.744	1.00 16.12	A
	ATOM	1915	CG	LEU A		34.050	22.320	28.974	1.00 14.73	A
	ATOM	1916		LEU A		35.192	21.935	29.912	1.00 14.56	Α
	ATOM	1917		LEU A		33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	. C	LEU A	312	34.181	25.189	29.774	1.00 16.61	Α

-	ATOM	1919	0	LEU	A 312	35.402	25.241	29.910	1.00 16.20	А
	ATOM	1920	N		A 313	33.515	25.949			
	ATOM	1921						28.908	1.00 16.20	A
			CA		A 313	34.207	26.907	28.058	1.00 15.37	Α
_	MOTA	1922	CB		A 313	33.216	27.648	27.130	1.00 16.42	A
5	ATOM	1923	CG1	VAL	A 313	33.915	28.796	26.426	1.00 16.93	Α
	MOTA	1924	CG2	VAL	A 313	32.644	26.672	26.103	1.00 17.88	A
	ATOM	1925	С		A 313	34.960	27.923	28.911	1.00 17.39	
	MOTA	1926	ō		A 313					A
						36.093	28.294	28.591	1.00 18.00	A
10	ATOM	1927	N		A 314	34.342	28.364	30.004	1.00 17.61	A
10	ATOM	1928	CA		A 314	34.986	29.331	30.885	1.00 20.43	A
	ATOM	1929	CB	GLU A	A 314	34.009	29.816	31.959	1.00 22.14	A
	ATOM	1930	CG	GLU A	A 314	32.800	30.550	31.396	1.00 26.52	A
	ATOM	1931	CD	GLU A		31.852	31.025	32.478	1.00 31.26	A
	ATOM	1932		GLU A						
15						31.580	30.246	33.417	1.00 33.48	A
13	MOTA	1933		GLU A		31.370	32.173	32.387	1.00 34.81	A
	ATOM	1934	C ·	GLU A		36.217	28.721	31.539	1.00 19.15	Α
	ATOM	1935	0	GLU A	A 314	37.134	29.433	31.934	1.00 21.47	A
	ATOM	1936	N	LYS A	A 315	36.245	27.400	31.651	1.00 19.51	А
	ATOM	1937	CA	LYS A		37.394	26.749	32.258	1.00 19.17	A
20	ATOM	1938	CB	LYS A		36.946				
20							25.514	33.043	1.00 18.84	A
	ATOM	1939	CG	LYS F		36.280	25.885	34.368	1.00 19.62	A
	MOTA	1940	CD	LYS A		35.653	24.696	35.073	1.00 19.22	Α
	MOTA	1941	CE	LYS F	315	35.070	25.095	36.427	1.00 21.00	Α
	ATOM	1942	NZ	LYS F	315	36.119	25.552	37.381	1.00 19.53	Α
25	ATOM	1943	С	LYS A	315	38.452	26.393	31.218	1.00 18.96	A
,	ATOM	1944	ō	LYS A		39.511	25.873	31.561		
	ATOM	1945		LEU A					1.00 19.85	A
			N			38.164	26.691	29.950	1.00 17.08	A
	ATOM	1946	CA	LEU P		39.102	26.429	28.854	1.00 16.41	A
	ATOM	1947	СВ	LEU F		38.414	25.636	27.738	1.00 13.81	A
30 -	ATOM	1948	CG	LEU F		38.028	24.201	28.115	1.00 14.39	A
	ATOM	1949	CD1.	LEU P	316	37.139	23.597	27.031	1.00 12.38	A
	MOTA	1950	CD2	LEU A	316	39.302	23.373	28.309	1.00 12.77	A A
	ATOM	1951	С	LEU A		39.652	27.743	28.290	1.00 17.12	A
	ATOM	1952	0	LEU A		40.851	27.860	28.023	1.00 16.53	
35	ATOM	1953	N	LEU A		38.780	28.729	28.105		A
	ATOM	1954	CA	LEU A		39.228			•	
							30.022	27.596	1.00 17.52	A
	ATOM	1955	СВ	LEU A		38.083	30.752	26.887	1.00 16.37	A
	ATOM	1956	CG	LEU A		37.448	29.973	25.727	1.00 18.81	A
	ATOM	1957		LEU A		36.415	30.851	25.018	1.00 16.47	A
40	ATOM	1958	CD2	LEU A	317	38.528	29.526	24.741	1.00 17.87	A
	ATOM	1959	С	LEU A	317	39.745	30.841	28.774	1.00 18.27	A
	ATOM	1960	Ō	LEU A			31.753	29.273	1.00 18.58	A
	ATOM	1961	N	VAL A		40.937	30.475	29.229	1.00 18.02	
	•						,			A
45	ATOM	1962	CA	VAL A		41.593	31.141	30.342	1.00 18.85	Α
45	ATOM	1963		VAL A		41.846	30.153	31.500	1.00 19.91	А
	ATOM	1964	CG1	VAL A	318	42.590	30.848	32.634	1.00 20.01	A
	ATOM	1965	CG2	VAL A	318	40.520	29.584	31.990	1.00 19.44	A
	ATOM	1966	С	VAL A	318	42.923	31.657	29.811	1.00 19.67	Α
	ATOM	1967	0	VAL A		43.690	30.902	29.208	1.00 18.26	A
50	ATOM	1968		LEU A		43.197	32.939	30.028	1.00 20.07	
50	ATOM	1969								A
				LEU A		44.436	33.533	29.538	1.00 20.98	A
	ATOM	1970		LEU A		44.521	35.002	29.968	1.00 21.64	A
	ATOM	1971		LEU A		43.418	35.908	29.408	1.00 24.38	A
	ATOM	1972	CD1	LEU A	319	43.606	37.332	29.935	1.00 23.28	A
55	ATOM	1973		LEU A		43.453	35.887	27.875	1.00 24.33	A
	ATOM	1974		LEU A		45.680	32.774	29.994	1.00 20.38	A
	ATOM	1975		LEU A		46.568	32.496	29.192	1.00 20.38	A
	ATOM	1976		ASP A		45.742				
	ATOM						32.440	31.280	1.00 20.22	A
	ATOM	1977	CA	ASP A	320	46.879	31.707	31.833	1.00 20.90	A

	ATOM	1978	CB	ASP .	A 320	46.842	31.760	33.365	1.00 20.76	A
	ATOM	1979	CG	ASP I	À 320	48.049	31.102	34.004	1.00 21.51	A
	ATOM	1980	OD1	ASP A	A 320	48.669	30.226	33.367	1.00 23.46	A
	ATOM	1981	OD2	ASP A	A 320	48.371	31.450	35.159	1.00 23.89	A
5	MOTA	1982	С	ASP A	A 320	46.814	30.247	31.367	1.00 20.06	A
	ATOM	1983	0	ASP A	A 320	45.988	29.476	31.840	1.00 20.54	A
	ATOM	1984	N	ALA A	A 321	47.700	29.876	30.451	1.00 20.68	A
	ATOM	1985	CA	ALA A	A 321	47.733	28.522	29.903	1.00 22.04	A
	MOTA	1986	CB	ALA A	A 321	48.860	28.411	28.881	1.00 20.75	A
10	ATOM	1987	С	ALA A	321	47.858	27.400	30.940	1.00 21.62	A
	ATOM	1988	0	ALA A	321	47.482	26.259	30.665	1.00 21.99	A
	ATOM	1989	N	THR A		48.372	27.715	32.127	1.00 20.89	A
	ATOM	1990	·CA	THR A		48.531	26.698	33.167	1.00 20.82	A
	ATOM	1991	CB	THR A	322	49.670	27.051	34.146	1.00 19.47	A
15	ATOM	1992	OG1	THR A	322	49.341	28.253	34.848	1.00 20.19	A
	ATOM	1993	CG2			50.981	27.249	33.394	1.00 21.59	A
	MOTA	1994	С	THR F		47.264	26.498	33.983	1.00 19.55	A
	ATOM	1995	0	THR A		47.235	25.673	34.894	1.00 21.13	A
	MOTA	1996	N	LYS F		46.216	27.248	33.661	1.00 19.33	A
20	MOTA	1997	CA	LYS F		44.962	27.122	34.392	1.00 21.20	A
	ATOM	1998	СВ	LYS A		44.580	28.460	35.030	1.00 23.75	A .
	ATOM	1999	CG	LYS A		45.562	28.933	36.084	1.00 28.45	A
	ATOM	2000	CD	LYS A		45.055	30.177	36.799	1.00 33.76	A
	ATOM	2001	CE	LYS A	323	46.087	30.678	37.802	1.00 36.15	A
25	ATOM	2002	NZ	LYS A		46.532	29.569	38.693	1.00 37.34	A
	ATOM	. 2003	С	LYS A		43.806	26.614	33.539	1.00 20.68	A
	MOTA	2004	0	LYS A		42.649	26.757	33.915	1.00 20.42	A
	ATOM	2005	N	ARG A	324	44.114	26.019	32.392	1.00 19.97	A
	ATOM	2006	CA	ARG A		43.060	25.494	31.531	1.00 17.98	A
30	ATOM	2007	CB	ARG A		43.461	25.609	30.061	1.00 15.95	A
	ATOM	2008	CG	ARG A		43.534	27.050	29.603	1.00 17.34	A
	ATOM	2009	CD	ARG A		43.996	27.194	28.172	1.00 19.80	A
	ATOM	2010	NE	ARG A		44.438	28.565	27.944	1.00 16.93	A
	ATOM	2011	CZ	ARG A		45.410	28.908	27.108	1.00 19.88	A
35	ATOM	2012	NH1	ARG A		46.045	27.978	26.398	1.00 14.58	A
	ATOM	2013		ARG A		45.774	30.181	27.015	1.00 16.51	, A
	MOTA	2014	С	ARG A		42.762	24.046	31.883	1.00 18.32	A
	ATOM	2015	0	ARG A		43.673	23.222	32.006	1.00 18.20	A
	ATOM	2016	N	LEU A		41.479	23.748	32.055	1.00 18.32	A
40	ATOM	2017	CA	LEU A		41.050	22.403	32.395	1.00 17.79	A
	ATOM	2018	СВ	LEU A		39.523	22.335	32.425	1.00 17.03	A
	ATOM	2019	CG	LEU A		38.896	21.125	33.116	1.00 15.91	A
	ATOM	2020	CD1	LEU A		39.392	21.048	34.557	1.00 15.93	A
	ATOM	2021		LEU A		37.375	21.255	33.084	1.00 16.56	A
45	ATOM	2022	С	LEU A		41.599	21.433	31.356	1.00 18.68	A
	ATOM	2023	0	LEU A		41.347	21.586	30.157	1.00 18.28	A
	ATOM	2024	N	GLY A		42.354	20.439	31.821	1.00 18.18	A
	ATOM	2025	CA	GLY A		42.931	19.462	30.915	1.00 16.36	A
	ATOM	2026		GLY A		44.443	19.558	30.807	1.00 19.15	A
50	ATOM	2027		GLY A		45.093	18.592	30.404	1.00 19.52	A
	ATOM	2028		CYS A		45.016	20.708	31.161	1.00 13.32	A
	ATOM	2029		CYS A		46.463	20.867	31.075	1.00 19.30	A
	ATOM	2030		CYS A		46.856	22.350	31.058	1.00 20.22	A
	ATOM	2031		CYS A		46.782	23.200	32.649	1.00 20.22	A
55	ATOM	2032		CYS A		47.169	20.157	32.228	1.00 20.22	A
•	ATOM	2033		CYS A		46.561	19.828	33.246	1.00 20.22	A
	ATOM	2033		GLU A		48.463	19.933	32.053	1.00 17.92	A
	ATOM	2035		GLU A		49.274	19.244	33.042	1.00 20.31	A
	ATOM	2036		GLU A		50.710	19.139	32.507	1.00 28.68	A
						20.710		52.501	2.00 20.00	Δ.

	ATOM	2037	CG	GLU A	328	50.754	18.367	31.175	1.00 38.24	A
	MOTA	2038	CD	GLU A	.328	52.067	18.500	30.414	1.00 43.23	A
	MOTA	2039	OE	L GLU A	328	52.535	19.643	30.218	1.00 46.22	A
	MOTA	2040	OE2	GLU A	328	52.618	17.459	29.991	1.00 44.90	A
5	ATOM	2041	·C	GLU A	328	49.234	19.876	34.435	1.00 22.11	Α.
	MOTA	2042	0	GLU A		49.147	19.161	35.437	1.00 20.27	A
	ATOM	2043	N	GLU A		49.276	21.204	34.506	1.00 18.40	A
	ATOM	2044	CA	GLU A		49.248	21.875	35.801	1.00 20.13	A
	ATOM	2045	СВ	GLU A		49.587	23.363	35.657	1.00 20.36	A
10	ATOM	2046	CG	GLU A		51.014	23.651	35.190	1.00 24.05	A
	ATOM	2047	CD	GLU A		51.191	23.518	33.688	1.00 25.93	A
	ATOM	2048	OE1			50.213	23.154	32.995	1.00 26.61	Ā
	ATOM	2049		GLU A		52.311	23.781	33.198	1.00 20.01	A
	ATOM	2050	C	GLU A		47.890	21.718	36.480	1.00 27.19	A
15	ATOM	2051	ŏ	GLU A		47.775	21.879	37.694	1.00 19.30	A
13	ATOM	2052	N	MET A		46.863	21.415	35.691	1.00 13.74	A
	ATOM	2053	CA	MET A		45.520	21.220	36.229	1.00 17.28	A
	ATOM	2054	CB	MET A		44.474	21.833	35.294	1.00 10.38	
	ATOM	2055	CG	MET A		44.460	23.365	35.234	1.00 17.65	A
20	ATOM	2056	SD	MET A		44.186	24.026	36.979	1.00 22.93	A
20	ATOM	2057	CE	MET A		42.435	24.026			A
	ATOM	2058	CE	MET A				37.186	1.00 24.69	A
	ATOM	2059	0	MET A		45.257	19.730	36.422	1.00 14.30	A
						44.127	19.304	36.629	1.00 15.39	A
25	MOTA	2060	N	GLU A		46.327	18.949	36.346	1.00 15.60	A
25	ATOM	2061	CA	GLU A		46.289	17.501	36.531	1.00 17.08	A
	ATOM	2062	CB	GLU A		45.607	17.155	37.862	1.00 17.00	A
	MOTA	2063	CG	GLU A		46.070	18.027	39.038	1.00 17.46	A
	ATOM	2064	CD			47.591	18.179	39.145	1.00 20.16	A
20	ATOM	2065		GLU A		48.034	19.073	39.896	1.00 21.39	A
30	ATOM	2066		GLU A		48.345	17.420	38.500	1.00 18.87	A
	ATOM	2067	C	GLU A		45.697	16.658	35.398	1.00 17.80	A
	MOTA	2068	0	GLU A		45.107	15.602	35.636	1.00 20.40	A
	ATOM	2069	N ·	GLY A		45.844	17.133	34.167	1.00 16.23	A
25	ATOM	2070	CA	GLY A		45.420	16.353	33.015	1.00 14.10	A
35	ATOM	2071	C	GLY A		43.982	16.154	32.596	1.00 13.54	A
	ATOM	2072	0	GLY A		43.063	16.864	33.017	1.00 11.96	A
	MOTA	2073	N	TYR A		43.804	15.141	31.750	1.00 14.37	A
	ATOM	2074	CA	TYR A		42.510	14.806	31.182	1.00 13.56	A
40	MOTA	2075	CB	TYR A		42.722	13.892	29.968	1.00 15.00	A
40	ATOM	2076	CG	TYR A		43.153	14.683	28.752	1.00 16.46	A
	ATOM ATOM	2077 2078	CD1			42.206	15.172	27.849	1.00 15.29	A
			CE1			42.573	16.002	26.794	1.00 13.42	A.
	ATOM	2079	CD2			44.490	15.039	28.561	1.00 14.91	A
15	ATOM	2080	CE2			44.872	15.877	27.499	1.00 14.87	A
45	ATOM	2081	CZ	TYR A		43.902	16.353	26.626	1.00 15.61	A
	ATOM	2082	ОН	TYR A		44.244	17.197	25.599	1.00 17.29	A
	ATOM	2083	C	TYR A		41.470	14.230	32.127	1.00 15.23	A
	ATOM	2084	0	TYR A		40.278	14.323	31.846	1.00 16.63	A
50	ATOM	2085	N	GLY A		41.907	13.650	33.244	1.00 15.50	A
_. 50	ATOM	2086	CA	GLY A		40.957	13.100	34.202	1.00 15.07	A
	ATOM	2087	C	GLY A		39.925	14.146	34.616	1.00 16.40	A
	ATOM	2088	0	GLY A		38.724	13.946	34.433	1.00 15.05	A
	ATOM	2089	N	PRO A		40.366	15.278	35.184	1.00 14.96	A
55	MOTA	2090	CD	PRO A		41.727	15.531	35.689	1.00 15.88	A
55	MOTA	2091	CA	PRO A		39.444		35.606	1.00 15.29	A
	ATOM	2092	CB	PRO A		40.383	17.397	36.178	1.00 13.19	A
	ATOM	2093	CG	PRO A		41.485	16.569	36.758	1.00 13.81	A
	ATOM	2094	C	PRO A		38.594	16.877	34.448	1.00 15.84	A
	ATOM	2095	0	PRO A	335	37.423	17.204	34.631	1.00 14.84	A

APOM 2098 CB LEU A 336 39.396 17.653 30.898 1.00 14.39 APOM 2099 CG LEU A 336 38.770 17.991 29.538 1.00 14.39 APOM 2100 CD1 LEU A 336 37.836 19.182 29.662 1.00 11.25 APOM 2100 CD1 LEU A 336 37.836 19.182 29.662 1.00 11.25 APOM 2100 CD1 LEU A 336 37.836 19.182 29.662 1.00 11.25 APOM 2100 CD2 LEU A 336 37.836 19.182 29.662 1.00 14.18 APOM 2100 CD2 LEU A 336 37.836 19.182 29.662 1.00 14.18 APOM 2100 CD2 LEU A 336 36.176 1.6.921 31.540 1.00 15.51 APOM 2104 CD2 LEU A 336 36.176 1.6.921 31.540 1.00 15.51 APOM 2106 CD2 LYS A 337 37.6624 15.225 31.592 1.00 17.23 APOM 2106 CD2 LYS A 337 37.293 12.900 30.921 1.00 17.39 APOM 2108 CD2 LYS A 337 39.213 11.892 29.592 1.00 24.76 APOM 2100 CD2 LYS A 337 39.213 11.892 29.592 1.00 24.76 APOM 2110 CD2 LYS A 337 39.213 11.892 29.592 1.00 24.76 APOM 2111 CD2 LYS A 337 39.577 09.560 29.189 1.00 24.76 APOM 2111 CD2 LYS A 337 34.674 10.96 32.342 1.00 17.33 APOM 2112 CD2 LYS A 337 34.656 13.652 29.997 1.00 25.65 APOM 2112 CD2 LYS A 337 34.656 13.652 29.997 1.00 15.63 APOM 2114 CD2 LYS A 337 34.656 13.652 29.997 1.00 14.42 APOM 2114 CD2 LYS A 337 34.456 13.652 29.997 1.00 15.63 APOM 2114 CD2 LYS A 337 34.456 13.652 32.990 1.00 14.42 APOM 2114 CD2 LYS A 337 34.456 13.652 32.990 1.00 14.42 APOM 2114 CD2 LYS A 337 34.456 13.652 32.990 1.00 14.42 APOM 2114 CD2 LYS A 338 34.999 14.395 34.674 1.00 17.52 APOM 2114 CD2 LYS A 338 34.674 1.00 17.52 APOM 2114 CD2 LYS A 338 34.674 1.00 17.52 APOM 2114 CD2 LYS A 338 34.674 1.00 17.52 APOM 2114 CD2 LYS A 339 33.486 LR.189 14.995 34.674 1.00 17.68 APOM 21.40 CD		ATOM ATOM	2096 2097	N CA	LEU A		39.184 38.450	16.971 17.465	33.257 32.094	1.00 16.12 1.00 15.52	. A A
ATOM 2009 CG LEU A 336 38.770 17.991 29.538 1.00 15.46 A A ATOM 2100 CD LEU A 336 39.884 18.285 28.528 1.00 14.112 A A ATOM 2102 C LEU A 336 39.884 18.285 28.528 1.00 14.112 A A ATOM 2103 C LEU A 336 37.321 16.508 31.714 1.00 15.28 A A ATOM 2104 N LYS A 337 37.640 15.225 31.592 1.00 17.22 A A ATOM 2105 C A LYS A 337 36.624 14.233 31.525 1.00 17.22 A A ATOM 2106 C B LYS A 337 37.660 15.225 31.592 1.00 17.22 A A ATOM 2106 C B LYS A 337 37.293 12.900 30.221 1.00 17.29 A A ATOM 2107 C LYS A 337 39.213 11.892 29.676 1.00 27.13 A A A ATOM 2109 CE LYS A 337 39.213 11.892 29.592 1.00 24.60 A A A A A A A A A A A A A A A A A A											
5 ATOM 2100 CD1 LEU A 336 37, 836 19.182 29.662 1.00 11.25 A ATOM 2101 CD2 LEU A 336 39.84 18.255 28.528 1.00 14.11 A A ATOM 2103 CD LEU A 336 37.321 16.508 31.714 1.00 16.28 A A ATOM 2104 N. LIS A 337 37.640 15.225 31.592 1.00 17.22 A A ATOM 2105 CA LIS A 337 37.640 15.225 31.592 1.00 17.22 A A ATOM 2106 CB LIS A 337 37.640 15.225 31.592 1.00 17.22 A A ATOM 2106 CB LIS A 337 37.640 15.225 31.592 1.00 17.23 A A ATOM 2106 CD LIS A 337 37.640 15.225 31.235 1.00 17.39 A A ATOM 2106 CD LIS A 337 39.213 11.892 29.676 1.00 22.31 A A ATOM 2108 CD LIS A 337 39.213 11.892 29.676 1.00 22.31 A A ATOM 2108 CD LIS A 337 39.213 11.892 29.676 1.00 24.76 A A ATOM 2110 NZ LIS A 337 39.213 11.892 29.592 1.00 24.76 A A ATOM 2110 NZ LIS A 337 39.10 9.560 28.897 1.00 24.76 A A ATOM 2110 NZ LIS A 337 34.656 13.652 32.090 1.00 14.42 A A A A A A A A A A A A A A A A A A A											
ATOM 2101 CDZ LEU A 336	•										
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ATOM 2114 CA ALA A 338 34.989 14.395 34.674 1.00 17.52 A ATOM 2115 CB ALA A 338 35.749 14.167 35.980 1.00 19.68 A ATOM 2116 C ALA A 338 35.749 14.167 35.980 1.00 19.68 A ATOM 2117 O ALA A 338 34.095 15.621 34.804 1.00 18.94 A ATOM 2118 N HIS A 339 34.262 16.596 33.918 1.00 19.22 A ATOM 2119 CA HIS A 339 33.456 16.596 33.918 1.00 19.28 A ATOM 2120 CB HIS A 339 33.865 18.819 32.949 1.00 19.28 A ATOM 2121 CG HIS A 339 33.865 18.819 32.949 1.00 19.28 A ATOM 2122 CD 2 HIS A 339 33.865 18.819 32.949 1.00 19.20 A ATOM 2122 CD 2 HIS A 339 33.549 21.299 33.649 1.00 19.20 A ATOM 2123 ND1 HIS A 339 33.549 21.299 33.649 1.00 19.20 A ATOM 2123 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2124 CEL HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2125 NEZ HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2126 C HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2126 C HIS A 339 31.507 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 17.448 33.845 1.00 19.13 A ATOM 2128 N PRO A 340 31.424 19.119 35.640 1.00 19.52 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.80 A ATOM 2130 CA PRO A 340 31.424 19.119 35.640 1.00 19.80 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2134 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2135 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2135 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2136 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2136 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2136 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2136 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 21		MOTA	2112	0			34.456				
20 ATOM 2115 CB ALA A 338 35.749 14.167 35.980 1.00 19.68 A A ATOM 2116 C ALA A 338 34.095 15.621 34.804 1.00 19.68 A ATOM 2117 O ALA A 338 33.252 15.667 35.695 1.00 18.83 A ATOM 2118 N HIS A 339 34.262 15.667 35.695 1.00 18.93 A ATOM 2119 CA HIS A 339 34.262 15.667 35.695 1.00 19.42 A ATOM 2119 CA HIS A 339 33.438 17.796 34.004 1.00 19.28 A ATOM 2120 CB HIS A 339 33.438 17.796 34.004 1.00 19.20 A ATOM 2121 CG HIS A 339 33.438 17.796 34.004 1.00 19.20 A ATOM 2121 CG HIS A 339 33.655 18.819 32.949 1.00 19.20 A ATOM 2122 CD2 HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 ND1 HIS A 339 31.606 21.576 32.896 1.00 22.79 A ATOM 2124 CEI HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 ND2 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2126 C HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2127 O HIS A 339 31.507 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 17.448 33.845 1.00 19.13 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.52 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.52 A ATOM 2130 CA PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 21.33 A ATOM 2137 CB PRE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PRE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PRE A 341 29.528 18.606 32.237 1.00 21.35 A ATOM 2137 CB PRE A 341 29.529 19.624 30.017 1.00 21.64 A ATOM 2137 CB PRE A 341 29.533 19.548 26.220 1.00 23.18 A ATOM 2140 CD2 PRE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2140 CD2 PRE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2140 CD2 PRE A 341 29.533 19.548 26.220 1.00 21.33 A ATOM 2140 CD2 PRE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CC2 PRE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2140 CD2 PRE A 341 29.533 19.549 29.550 1.00 20.37 A ATOM 2145 CC2 PRE A 341 29.553 19.560 29.389 1.		ATOM	2113	N	ALA A	338					
ATOM 2116 C ALA A 338 34.095 15.621 34.804 1.00 18.83 A A ATOM 2117 O ALA A 338 33.252 15.687 35.695 1.00 18.94 A ATOM 2118 N HIS A 339 34.262 16.596 33.918 1.00 19.42 A ATOM 2119 CA HIS A 339 33.463 17.796 34.004 1.00 19.28 A ATOM 2121 CG HIS A 339 33.463 17.796 34.004 1.00 19.28 A ATOM 2121 CG HIS A 339 33.865 18.819 32.949 1.00 19.20 A ATOM 2122 CD2 HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2122 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2125 NEZ HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NEZ HIS A 339 31.506 22.179 33.525 1.00 21.98 A ATOM 2126 C HIS A 339 31.507 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.52 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2133 C PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2133 C PRO A 340 29.630 17.900 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 19.20 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 20.52 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 21.42 A ATOM 2135 C PRO A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2135 C PRO A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.64 A ATOM 2136 C PHE A 341 29.533 19.548 26.220 1.00 23.18 A ATOM 2136 C PHE A 341 29.503 19.548 26.220 1.00 23.18 A ATOM 2140 CD2 PHE A 341 29.503 19.548 26.220 1.00 23.31 A ATOM 2141 C PHE A 341 29.505 19.548 26.220 1.00 23.31 A ATOM 2141 C PHE A 341 29.505 19.548 26.220 1.00 23.31 A ATOM 2141 C PHE A 341 29.505 19.548 26.220 1.00 23.31 A ATOM 2144 C PHE A 341 29.505 19.548 26.220 1.00 23.31 A ATOM		ATOM	2114	CA	ALA A	338	34.989	14.395			
ATOM 2117 O ALA A 338 33.252 15.687 35.695 1.00 18.94 A ATOM 2118 N HIS A 339 34.262 16.596 33.918 1.00 19.42 A ATOM 2119 CA HIS A 339 34.262 16.596 33.918 1.00 19.42 A ATOM 2120 CB HIS A 339 33.438 17.796 34.004 1.00 19.28 A ATOM 2121 CG HIS A 339 33.465 18.819 32.949 1.00 19.20 A ATOM 2121 CG HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 33.549 21.299 33.649 1.00 18.95 A ATOM 2122 CD2 HIS A 339 33.549 21.299 33.649 1.00 19.20 A ATOM 2123 ND1 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2124 CE1 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2126 C HIS A 339 31.507 17.448 33.845 1.00 19.10 A ATOM 2126 C HIS A 339 31.507 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.577 16.576 33.611 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2130 CA PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.52 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 28.985 18.606 32.237 1.00 21.42 A ATOM 2135 C PRO A 341 28.985 18.606 32.237 1.00 21.42 A ATOM 2135 C PRO A 341 28.985 18.606 32.237 1.00 21.42 A ATOM 2136 CA PHE A 341 28.985 18.606 32.237 1.00 21.42 A ATOM 2137 CB PHE A 341 28.985 18.606 32.237 1.00 21.57 A ATOM 2136 CA PHE A 341 29.529 18.606 32.237 1.00 21.42 A ATOM 2137 CB PHE A 341 29.533 19.548 22.237 1.00 21.57 A ATOM 2134 CC PHE A 341 29.539 19.624 30.017 1.00 21.64 A ATOM 2137 CB PHE A 341 29.539 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.539 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.539 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.539 19.624 30.017 1.00 21.64 A ATOM 2146 CP PHE A 341 29.539 19.548 26.220 1.00 21.33 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2146 CP PHE A 341 29.553 19.548 26.220 1.00 21.84 A A	20	MOTA	2115	CB	ALA A	338	35.749	14.167	35.980		
ATOM 2118 N HIS A 339 34.262 16.596 33.918 1.00 19.42 A ATOM 2119 CA HIS A 339 33.438 17.796 34.004 1.00 19.28 A ATOM 2120 CB HIS A 339 33.438 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 33.585 18.819 32.949 1.00 19.20 A ATOM 2122 CD2 HIS A 339 33.548 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2124 CE1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2125 NEZ HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NEZ HIS A 339 31.506 21.576 32.896 1.00 21.98 A ATOM 2125 NEZ HIS A 339 31.507 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.957 17.448 33.845 1.00 19.13 A ATOM 2128 N PRO A 340 31.494 19.119 35.640 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.001 17.834 33.176 1.00 19.20 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 20.74 A ATOM 2133 C PRO A 340 29.001 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2138 CG PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2138 CG PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2138 CG PHE A 341 29.528 18.606 32.237 1.00 21.53 A ATOM 2138 CG PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2137 CB PHE A 341 29.528 18.606 32.237 1.00 21.53 A ATOM 2134 CC PHE A 341 29.528 18.606 32.237 1.00 21.53 A ATOM 2138 CG PHE A 341 29.528 18.606 32.237 1.00 21.53 A ATOM 2139 CD PHE A 341 29.533 19.548 26.220 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.528 18.606 32.237 1.00 21.84 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 21.84 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 21.84 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1		ATOM	2116	С	ALA A	338	34.095				
ATOM 2120 CB HIS A 339 33.438 17.796 34.004 1.00 19.28 A A ATOM 2121 CG HIS A 339 33.865 18.819 32.949 1.00 19.20 A A ATOM 2122 CG HIS A 339 33.865 18.819 32.949 1.00 19.20 A A ATOM 2122 ND1 HIS A 339 33.549 21.299 33.649 1.00 18.95 A ATOM 2123 ND1 HIS A 339 31.549 21.299 33.649 1.00 18.95 A ATOM 2123 ND1 HIS A 339 31.800 20.340 32.612 1.00 19.10 A ATOM 2124 CEI HIS A 339 31.800 20.340 32.612 1.00 19.10 A A ATOM 2125 NE2 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2126 C HIS A 339 31.506 21.576 32.896 1.00 21.98 A ATOM 2127 O HIS A 339 31.597 16.576 33.805 1.00 21.98 A ATOM 2128 N PRO A 340 31.597 16.576 33.845 1.00 19.13 A ATOM 2128 N PRO A 340 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2133 C PRO A 340 29.630 17.900 34.569 1.00 20.74 A ATOM 2133 C PRO A 340 29.630 17.900 34.569 1.00 20.74 A ATOM 2133 C PRO A 340 29.630 17.900 34.569 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2134 O PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2136 CA PHE A 341 29.739 19.624 30.017 1.00 21.42 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.43 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.237 1.00 23.58 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.237 1.00 23.58 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.237 1.00 23.54 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.290 1.00 23.35 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.290 1.00 23.54 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.290 1.00 23.54 A ATOM 2140 CD2 PHE A 341 29.553 19.548 26.290 1.00 23.55 A ATOM 2140 CD2 PHE A 341 29.555 17.226 30.237 1.00 23.54 A ATOM 2145 CD2 PHE A 341 29.555 17.226 30.077		MOTA	2117	0	ALA A	338					
25 ATOM 2121		ATOM	2118	N	HIS A	339	34.262	16.596	33.918		
ATOM 2121 CG HIS A 339 33.163 20.134 33.074 1.00 20.26 A ATOM 2122 CD2 HIS A 339 33.549 21.299 33.649 1.00 18.95 A ATOM 2123 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2124 CE1 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NE2 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NE2 HIS A 339 31.506 21.576 32.896 1.00 19.13 A ATOM 2126 C HIS A 339 31.597 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2133 C PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.088 32.955 1.00 21.42 A ATOM 2133 C PRO A 340 29.091 17.088 32.955 1.00 21.42 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 19.20 A ATOM 2133 C PRO A 340 29.090 17.088 32.955 1.00 21.42 A ATOM 2135 C PRO A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2135 C PRO A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2135 C PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2134 C PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2134 C C PHE A 341 29.533 19.548 26.220 1.00 23.18 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.553 15.82 28.971 1.00 12.84 A ATOM 2144 C PHE A 341 29.553 15.82 28.971 1.00 17.05 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2145 C PHE A 341 29.555 17.226 30.237 1.00 23.01 A ATOM 2145 C PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 214		ATOM	2119	CA	HIS A	339	33.438				
ATOM 2122 CD2 HIS A 339 33.549 21.299 33.649 1.00 18.95 A ATOM 2123 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2124 CE1 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NE2 HIS A 339 32.500 22.179 33.525 1.00 21.98 A ATOM 2126 C HIS A 339 31.957 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.957 17.448 33.845 1.00 19.13 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.08 A ATOM 2129 CD PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2132 CG PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 28.049 17.088 32.955 1.00 22.48 A ATOM 2133 C PRO A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2136 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.58 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.553 17.266 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 17.266 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2145 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2145 CB PHE A 342 30.21 15.085 30.077 1.00 23.01 A ATOM 21	25	ATOM	2120	CB	HIS A	339	33.865	18.819	32.949		
ATOM 2123 ND1 HIS A 339 31.880 20.340 32.612 1.00 19.10 A ATOM 2124 CE1 HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NE2 HIS A 339 32.500 22.179 33.525 1.00 21.98 A ATOM 2126 C HIS A 339 31.507 21.748 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.13 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.80 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2132 CG PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 17.884 33.176 1.00 19.20 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2140 CD2 PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2141 CE1 PHE A 341 29.739 19.624 30.017 1.00 21.83 A ATOM 2141 CE1 PHE A 341 29.739 19.624 30.017 1.00 21.83 A ATOM 2141 CE1 PHE A 341 29.533 19.431 27.522 1.00 23.54 A ATOM 2141 CE1 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2145 CB PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2146 N PHE A 342 30.014 16.422 30.640 1.00 17.05 A ATOM 2147 CA PHE A 342 30.017 17.00 29.51 A ATOM 2148 CB PHE A 342 30.017 17.08 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 30.010 15.987 27.652 1.00 17.78 A ATOM	•	ATOM	2121	CG	HIS A	339	33.163	20.134	33.074		
ATOM 2124 CEI HIS A 339 31.506 21.576 32.896 1.00 22.19 A ATOM 2125 NE2 HIS A 339 32.500 22.179 33.525 1.00 21.98 A ATOM 2126 C HIS A 339 31.597 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2140 CD2 PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2141 CEI PHE A 341 29.207 19.740 28.623 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.84 A ATOM 2145 O PHE A 341 29.553 19.548 26.220 1.00 23.54 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 23.54 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.57 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CDI PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM		ATOM	2122	CD2	HIS A	339		21.299	33.649		
30 ATOM 2125 NE2 HIS A 339 32.500 22.179 33.525 1.00 21.98 A ATOM 2126 C HIS A 339 31.957 17.448 33.645 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.74 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 19.20 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 20.74 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 22.48 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 23.18 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2141 CE1 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2147 CA PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2146 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2147 CA PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 21.83 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CG PHE A 342 30.034 16.422 30.640 1.00 17.05 A ATOM 2149 CG PHE A 342 32.31710 14.809 29.850 1.00 17.78 A ATOM 2149 CG PHE A 342 32.300 15.987 27.6652 1.00 17.78 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.010 15.987 27.6652 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.6652 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.6652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 32.00 16.867 26.811 1.00		ATOM	2123	ND1	HIS A	339	31.880	20.340		1.00 19.10	A
ATOM 2126 C HIS A 339 31.957 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.08 A ATOM 2129 CD PRO A 340 31.079 18.125 34.606 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2132 CG PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 23.58 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2143 CZ PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2143 CZ PHE A 341 29.533 19.548 26.220 1.00 23.23 A ATOM 2144 C PHE A 341 28.288 19.980 25.998 1.00 23.23 A ATOM 2147 CA PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 21.83 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.021 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 30.034 16.542 30.677 1.00 23.01 A ATOM 2148 CB PHE A 342 30.034 16.542 30.677 1.00 23.01 A ATOM 2149 CG PHE A 342 33.387 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.308 15.812 28.971 1.00 17.05 A ATOM 2152 CE1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.010 15.987 27.662 1.00 17.75 A ATOM 2152 CE1 PHE A 342 32.010 15.987 27.662 1.00 17.765 A		ATOM	2124	CE1	HIS A	339	31.506	21.576	32.896		
ATOM 2127 O HIS A 339 31.957 17.448 33.845 1.00 19.13 A ATOM 2127 O HIS A 339 31.597 16.576 33.061 1.00 19.52 A ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2132 CG PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PRE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.528 18.606 30.886 1.00 21.57 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2136 CA PHE A 341 29.207 19.740 28.613 1.00 22.58 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2141 CE1 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.266 30.237 1.00 21.84 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.887 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 32.010 15.887 27.652 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.010 15.886 26.617 1.00 17	30	ATOM	2125	NE2	HIS A	339	32.500	22.179	33.525	1.00 21.98	A
ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A A ATOM 2130 CA PRO A 340 29.630 17.900 35.640 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 36.454 1.00 20.74 A ATOM 2132 CG PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 28.049 17.088 32.955 1.00 22.48 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A A ATOM 2135 CA PHE A 341 29.528 18.606 32.237 1.00 21.33 A A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A A ATOM 2139 CD1 PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 27.410 20.292 27.082 1.00 21.95 A ATOM 2142 CE2 PHE A 341 29.533 19.548 27.522 1.00 23.54 A ATOM 2144 C PHE A 341 29.533 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.533 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.533 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 23.23 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 23.23 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 23.23 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 23.23 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 23.23 A ATOM 2144 C PHE A 342 30.034 16.422 30.640 1.00 20.551 A ATOM 2144 CB PHE A 342 30.034 16.422 30.640 1.00 20.551 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.551 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.551 A ATOM 2148 CB PHE A 342 30.341 16.422 30.640 1.00 20.551 A ATOM 2149 CG PHE A 342 30.034 16.422 30.640 1.00 20.551 A ATOM 2145 CD PHE A 342 30.3487 16.584 29.850 1.00 17.05 A ATOM 2145 CD PHE A 342 30.3487 16.584 29.450 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.300 15.585 20.640 1.00 10.00 17.05 A ATOM 2150 CD1 PHE A 342 32.700 16.867 26.811 1.00 17.05 A ATOM 2152 CE1 PHE A 342 32.700 16.867 26.811 1.00 17.05 A ATOM 2152 CE1 PHE A 342 32.700 16.86		ATOM	2126	С	HIS A	339	31.957	17.448	33.845		
ATOM 2128 N PRO A 340 31.079 18.125 34.606 1.00 19.80 A ATOM 2129 CD PRO A 340 31.424 19.119 35.640 1.00 19.08 A ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.630 17.900 34.569 1.00 20.74 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.42 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 23.18 A ATOM 2139 CD1 PHE A 341 29.739 19.624 30.017 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 23.18 A ATOM 2140 CD2 PHE A 341 27.410 20.292 27.082 1.00 21.95 A ATOM 2141 CE1 PHE A 341 29.533 19.548 27.522 1.00 21.95 A ATOM 2143 CZ PHE A 341 29.533 19.548 27.522 1.00 21.83 A ATOM 2144 C PHE A 341 29.533 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.533 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.553 19.548 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 20.37 A ATOM 2144 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.334 16.422 30.640 1.00 23.01 A ATOM 2145 CB PHE A 342 30.341 16.422 30.640 1.00 23.01 A ATOM 2145 CB PHE A 342 30.334 16.422 30.640 1.00 23.01 A ATOM 2145 CB PHE A 342 30.341 16.422 30.640 1.00 20.51 A ATOM 2145 CB PHE A 342 30.341 16.422 30.640 1.00 10.00 10.51 A ATOM 2145 CB PHE A 342 30.341 16.422 30.640 1.00 10.00 17.78 A ATOM 2145 CB PHE A 342 30.010 15.987 27.652 1.00		ATOM	2127	0	HIS A	339	31.597	16.576	33.061		
ATOM 2130 CA PRO A 340 29.630 17.900 34.569 1.00 20.52 A ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2132 CG PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.090 17.834 33.176 1.00 21.42 A ATOM 2134 O PRO A 340 28.049 17.088 32.955 1.00 22.48 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.528 18.610 30.886 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2141 CE1 PHE A 341 27.903 20.171 28.382 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.739 19.548 26.220 1.00 21.83 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 23.23 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 23.23 A ATOM 2145 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A A ATOM 2145 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A A A A A A A A A		ATOM	2128	N	PRO A	340	31.079		34.606		
ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2132 CG PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2134 O PRO A 340 28.049 17.088 32.955 1.00 22.48 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.739 19.624 30.017 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2139 CD1 PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 21.95 A ATOM 2143 CZ PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2145 O PHE A 341 28.228 19.980 25.998 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CG PHE A 342 30.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.702 16.867 26.811 1.00 15.72 A ATOM 2150 CD1 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2150 CD1 PHE A 342 32.702 16.867 26.811 1.00 17.45 A		ATOM	2129	CD	PRO A	340	31.424	19.119	35.640		
ATOM 2131 CB PRO A 340 29.091 19.058 35.396 1.00 20.74 A ATOM 2132 CG PRO A 340 30.146 19.207 36.454 1.00 19.20 A ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2134 O PRO A 340 28.049 17.088 32.955 1.00 22.48 A ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 29.528 18.606 32.237 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.555 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2146 N PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 17.78 A ATOM 2152 CE1 PHE A 342 33.487 16.534 29.450 1.00 17.78 A ATOM 2152 CE1 PHE A 342 33.487 16.534 29.450 1.00 17.78 A ATOM 2153 CE2 PHE A 342 33.487 16.534 29.450 1.00 17.78 A	35	ATOM	2130	CA	PRO A	340	29.630	17.900	34.569		
ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2134 O PRO A 340 28.049 17.088 32.955 1.00 22.48 A 40 ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 28.985 18.610 30.886 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 23.18 A ATOM 2140 CD2 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 21.95 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CG PHE A 342 30.021 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 32.31710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 17.45			2131	СВ	PRO A	340	29.091	19.058	35.396	1.00 20.74	
ATOM 2133 C PRO A 340 29.000 17.834 33.176 1.00 21.42 A ATOM 2134 O PRO A 340 28.049 17.088 32.955 1.00 22.48 A 40 ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2136 CA PHE A 341 28.985 18.610 30.886 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A 45 ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.317 10.5987 27.652 1.00 17.78 A ATOM 2150 CD2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2151 CD2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45		ATOM	2132	CG.	PRO A	340	30.146	19.207	36.454		A
ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 29.055 17.226 30.237 1.00 21.83 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2146 N PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2149 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2151 CD2 PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A			2133	С	PRO A	340	29.000	17.834	33.176		
ATOM 2135 N PHE A 341 29.528 18.606 32.237 1.00 21.33 A ATOM 2137 CB PHE A 341 28.985 18.610 30.886 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 21.95 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.301 15.987 27.652 1.00 17.78 A ATOM 2150 CD1 PHE A 342 32.301 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 17.45 A		ATOM	2134	0	PRO A	340	28.049	17.088	32.955		A
ATOM 2136 CA PHE A 341 28.985 18.610 30.886 1.00 21.57 A ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2144 C PHE A 341 29.553 19.548 26.220 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2145 O PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2146 N PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.021 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2151 CD2 PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.702 16.867 27.652 1.00 17.78 A ATOM 2153 CE2 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A	40		2135	N	PHE A	341	29.528	18.606	32.237		
ATOM 2137 CB PHE A 341 29.739 19.624 30.017 1.00 21.64 A ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A 45 ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A ATOM 2145 C PHE A 341 28.232 16.896 29.389 1.00 23.23 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2151 CD2 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A			2136	CA	PHE A	341	28.985	18.610	30.886		A
ATOM 2138 CG PHE A 341 29.207 19.740 28.613 1.00 23.18 A ATOM 2139 CD1 PHE A 341 27.903 20.171 28.382 1.00 22.58 A 45 ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.398 15.812 28.971 1.00 17.78 A ATOM 2151 CD2 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A			2137	CB	PHE A	341	29.739	19.624	30.017		
45 ATOM 2140 CD2 PHE A 341 30.013 19.431 27.522 1.00 21.95 A ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2148 CB PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2149 CG PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 18.08 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A		ATOM	2138	CG	PHE A	341	29.207	19.740			
ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 18.08 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A		ATOM	2139	CD1	PHE A	341					
ATOM 2141 CE1 PHE A 341 27.410 20.292 27.082 1.00 23.54 A ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A	45		2140	CD2	PHE A	341	30.013	19.431			A
ATOM 2142 CE2 PHE A 341 29.533 19.548 26.220 1.00 21.83 A ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 18.08 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A			2141	CE1	PHE A	341	27.410	20.292	27.082		A
ATOM 2143 CZ PHE A 341 28.228 19.980 25.998 1.00 23.23 A ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A							29.533	19.548	26.220		
ATOM 2144 C PHE A 341 29.055 17.226 30.237 1.00 21.84 A 50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A			2143	CZ	PHE A	341	28.228	19.980	25.998		
50 ATOM 2145 O PHE A 341 28.232 16.896 29.389 1.00 20.37 A ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A			2144	С	PHE A	341	29.055	17.226	30.237		A
ATOM 2146 N PHE A 342 30.034 16.422 30.640 1.00 20.51 A ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A	50			0	PHE A	341	28.232	16.896	29.389	1.00 20.37	
ATOM 2147 CA PHE A 342 30.221 15.085 30.077 1.00 23.01 A ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A				N			30.034	16.422	30.640	1.00 20.51	
ATOM 2148 CB PHE A 342 31.710 14.809 29.850 1.00 18.00 A ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A				CA	PHE A	342	30.221	15.085	30.077	1.00 23.01	A
ATOM 2149 CG PHE A 342 32.398 15.812 28.971 1.00 17.05 A ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A							31.710	14.809	29.850		
55 ATOM 2150 CD1 PHE A 342 32.010 15.987 27.652 1.00 17.78 A ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A							32.398	15.812	28.971		
ATOM 2151 CD2 PHE A 342 33.487 16.534 29.450 1.00 15.72 A ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A	55							15.987	27.652		A
ATOM 2152 CE1 PHE A 342 32.702 16.867 26.811 1.00 18.08 A ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A							33.487	16.534	29.450		
ATOM 2153 CE2 PHE A 342 34.184 17.414 28.617 1.00 17.45 A							32.702	16.867	26.811		
00 000 00 000 1 00 1 EC - 7								17.414			A
							33.790	17.578	27.298	1.00 16.56	Α

								•				
	MOTA	2155	С	PHE	A	342	29.679	13.972	30.976	1.00 2	24.95	A
	ATOM	2156	0	PHE	Α	342	30.002	12.798	30.777	1.00 2	23.95	A
	ATOM	2157	N	GLU	Α	343	28.861	14.333	31.958	1.00 2	27.35	Α
	MOTA	2158	CA	GLU	Α	343	28.325	13.349	32.897	1.00 3	30.28	A
5	ATOM	2159	CB.	GLU	Α	343	27.187	13.964	33.716	1.00 3	32.20	A
	ATOM	2160	CG	GLU			26.581	12.991	34.714	1.00 3	9.71	A
	ATOM	2161	CD			343	25.628	13.661	35.688	1.00 4		A
	ATOM	2162		GLU			24.661	14.314	35.234	1.00 4		A
	ATOM	2163		GLU			25.847	13.526	36.911	1.00 4		A
10	ATOM	2164	C			343	27.852	12.017	32.305	1.00 2		A
10	ATOM	2165	Ö	GLU			28.225	10.952	32.800	1.00 3		A
	ATOM	2166	N ·	SER			27.037	12.067	31.258	1.00 2		A
		2167	CA	SER			26.520	10.838	30.656	1.00 2		A
	MOTA	2168	CB	SER			25.129	11.089	30.050	1.00 2		A
15	MOTA						25.123	11.942	28.940	1.00 2		A
15	ATOM	2169	OG	SER						1.00 3		A
	ATOM	2170	C	SER			27.407	10.214	29.577			
	ATOM	2171	0	SER			26.987	9.281	28.900	1.00 2		A
	MOTA	2172	N			345	28.627	10.715	29.419	1.00 2		A
	MOTA	2173	CA	VAL			29.534	10.183	28.402	1.00 2		A
20	MOTA	2174	CB	VAL			30.565	11.256	27.950	1.00 2		A
	MOTA	2175		VAL			31.589	10.631	26.995	1.00 2		A
	ATOM	2176		VAL			29.854	12.418	27.275	1.00 2		A
	MOTA	2177	С	VAL			30.326	8.957	28.855	1.00 2		A
	MOTA	2178	0	VAL			30.876	8.930	29.960	1.00 2		A
25	MOTA	2179	N	THR	Α	346	30.374	7.942	27.997	1.00 2		A
	MOTA	2180	CA	THR	А	346	31.153	6.740	28.272	1.00 2		A
	ATOM	2181	CB	THR	Α	346	30.391	5.455	27.857	1.00 2		Α
	ATOM	2182	OG1	THR	Α	346	29.248	5.284	28.706	1.00 2		A
	ATOM	2183	CG2	THR	A	346	31.289	4.231	27.990	1.00 2		A
30	MOTA	2184	С	THR	A	346	32.383	6.945	27.385	1.00 2	3.43	A
	ATOM	2185	0	THR	Α	346	32.306	6.827	26.160	1.00 2	4.50	A
	ATOM ·	2186	N	TRP	Α	347	33.508	7.270	28.013	1.00 2	2.98	A
	ATOM	2187	CA	TRP	Α	347	34.744	7.569	27.300	1.00 2	3.81	A
	ATOM	2188	СВ	TRP	Α	347	35.683	8.352	28.219	1.00 2	2.54	Α
35	ATOM	2189	CG	TRP	Α	347	35.128	9.658	28.693	1.00 2	0.61	A
	ATOM	2190	CD2	TRP	Α	347	35.257	10.927	28.040	1.00 1	9.11	· A
	ATOM	2191	CE2	TRP	Α	347	34.581	11.881	28.838	1.00 1	8.39	Α
	ATOM	2192	CE3	TRP	Α	347	35.878	11.351	26.858	1.00 1	8.16	A
	ATÓM	2193	CD1	TRP	Α	347	34.397	9.883	29.828	1.00 1	8.35	Α
40	ATOM	2194	NE1			347	34.065	11.218	29.923	1.00 1	9.51	A
	ATOM	2195	CZ2			347	34.510	13.234	28.491	1.00 1	6.88	A
	ATOM	2196	CZ3				35.808	12.701	26.511	1.00 1	7.23	Α
	ATOM	2197		TRP			35.127	13.624	27.327	1.00 1	8.16	A
	ATOM	2198	С	TRP			35.538	6.429	26.675	1.00 2	5.79	Α
45	ATOM	2199	ō	TRP			36.304	6.654	25.742	1.00 2	4.67	A
.5	ATOM	2200	N	ALA			35.360	5.215	27.183	1.00 2		A
	ATOM	2201	CA	ALA			36.116	4.063	26.697	1.00 2		A
	ATOM	2202	CB	ALA			35.899	2.869	27.636	1.00 2		А
	ATOM	2203	C	ALA			35.895	3.620	25.256	1.00 2		A
50	ATOM	2204	Ö	ALA			36.830	3.148	24.613	1.00 2		A
50	ATOM	2205	N	ASN			34.682	3.769	24.735	1.00 2		A
	ATOM	2205	CA	ASN			34.418	3.310	23.375	1.00 2		A
							33.700	1.962	23.444	1.00 2		A
	ATOM	2207	CB	ASN				2.088	24.013	1.00 2		A
55	MOTA	2208	CG OD1	ASN			32.299	2.942	24.013	1.00 3		A
55	ATOM	2209		ASN			32.045		23.553	1.00 3		A
	MOTA	2210		ASN			31.386	1.237		1.00 2		A
	ATOM	2211	C	ASN			33.599	4.265	22.509	1.00 2		A
	ATOM	2212	0	ASN			32.669	3.843	21.819			A
	ATOM	2213	N	LEU	A	350	33.947	5.543	22.518	1.00 2	. 4 . 4 3	А

									*			,
	ATOM	2214	CA	LEU A	350	33	3.203	6.510	21.721	1.00	23.14	A
	ATOM	2215	СВ	LEU A	350	33	3.837	7.898	21.848	1.00	23.22	A
	ATOM	2216	CG	LEU A			3.659	8.605	23.191		21.05	A
	ATOM	2217		LEU A			1.646	9.756	23.293		19.36	A
5	ATOM	2218		LEU A			2.220	9.094	23.319		18.78	A
3				LEU A			3.082	6.152	20.240		22.60	A
	ATOM	2219	C	LEU A					19.650			
-	ATOM	2220	0				2.011	6.296			21.15	A
	MOTA	2221	N	HIS A			1.165	5.689	19.627		23.13	A
	ATOM	2222	CA	HIS A			1.089	5.387	18.204		27.83	Ä
10	ATOM	2223	СВ	HIS A			5.506	5.325	17.596		29.36	A
	ATOM	2224	CG	HIS A		36	5.082	3.950	17.493	1.00	32.07	A
	ATOM	2225	CD2	HIS A	351	36	5.611	3.128	18.431	1.00	32.39	Α
	ATOM	2226	ND1	HIS A	351	36	5.197	3.285	16.291	1.00	33.02	A
	ATOM	2227	CE1	HIS A	351	36	5.775	2.113	16.493	1.00	33.58	A
15	ATOM	2228		HIS A		37	7.036	1.992	17.782	1.00	31.76	A
	MOŤA	2229	С	HIS A			3.258	4.144	17.874	1.00	28.12	A
	ATOM	2230	Ö	HIS A			3.015	3.847	16.707		29.49	A
	ATOM	2231	N	GLN A			2.800	3.442	18.908		29.28	Ą
		2232	CA	GLN A			1.963	2.255	18.726		29.67	Ā
20	ATOM			GLN A			2.366		19.694		30.56	A
20	ATOM	2233	CB									- A
	ATOM	2234	CG	GLN A			3.169	0.041	19.041		30.88	
	MOTA	2235	CD	GLN A			1.493	-0.186	19.729		31.21	A
	ATOM	2236		GLN A			1.541	-0.450	20.928		30.76	A
	ATOM	2237		GLN A			5.578	-0.084	18.971		32.30	A
25	MOTA	2238	С	GLN A			0.504	2.638	18.963		30.42	A
	MOTA	2239	0	GLN A	352		9.595	1.831	18.770		29.01	A
	ATOM	2240	Ν.	GLN A	353	30	0.290	3.875`	19.397		27.64	A
	MOTA	2241	CA	GLN A	. 353	28	3.948	4.365	19.652	1.00	27.42	A
-	ATOM	2242	CB	GLN A	353	28	3.977	5.401	20.775	1.00	25.77	A
30	MOTA	2243	CG	GLN A	353	29	9.408	4.837	22.115	1.00	27.34	Α
	ATOM	2244	CD	GLN A	353	29	9.638	5.914	23.156	1.00	27.19	A
	ATOM	2245	OE1	GLN A	353	28	3.875	6.872	23.252	1.00	28.29	A
•	ATOM	2246		GLN A			0.687	5.753	23.951	1.00	28.79	A
	ATOM	2247	C	GLN A			3.375	4.989	18.385	1.00	29.00	A
35	ATOM	2248	ō	GLN A			9.118	5.455	17.516		29.14	A
33	ATOM	2249	N	THR A			7.053	4.984	18.276		27.31	A
	ATOM	2250	CA	THR A			5.390	5.568	17.119		27.85	A
	ATOM	2251	CB	THR A			1.991	4.941	16.904		30.69	A
		2252					5.132	3.532	16.665		30.07	A
40	ATOM			THR A			1.289	5.585	15.709		29.58	A
40	ATOM	2253		THR A			5.244	7.062	17.376		26.85	A
	ATOM	2254 .	С	THR A							25.77	A
•	ATOM	2255	0	THR A			5.592	7.475	18.329		27.22	A
	ATOM	2256	N	PRO A			5.867	7.898	16.533			A
	ATOM	2257	CD	PRO A			7.792	7.588	15.431		25.89	
45	ATOM	2258	CA	PRO A			5.763	9.346	16.734		27.23	A
	ATOM	2259	СВ	PRO A			7.625	9.915	15.609		24.91	A
	ATOM	2260	CG	PRO A	355		3.643	8.838	15.385		25.54	A
	ATOM	2261	С	PRO A	355		5.322	9.837	16.641		28.07	A
	ATOM	2262	0	PRO A	355	24	1.548	9.364	15.810		27.24	A
50	MOTA	2263	N	PRO A	356	24	1.941	10.792	17.500	1.00	28.28	A
	ATOM	2264	CD	PRO A		25	5.752	11.560	18.462	1.00	28.31	A
	ATOM	2265	CA	PRO A		23	3.572	11.306	17.448	1.00	28.44	A
	ATOM	2266	СВ	PRO · A			3.539	12.301	18.604		28.11	A
	ATOM	2267	CG	PRO A			1.946	12.832	18.612		26.86	A
55	ATOM	2268	C	PRO A			3.363	11.978	16.097		29.25	A
55		2269	0	PRO A			1.304	12.537	15.529		27.27	A
	ATOM			ALA A			2.143	11.910	15.575		30.45	A
	ATOM .	2270	N C7				L.848	12.521	14.287		32.81	A
	ATOM	2271	CA	ALA A							31.99	A
	MOTA	2272	CB	ALA A	. 35/	20).507	12.019	13.757	1.00	31.33	M

	ATOM	2273	С	ALA	A	357		21.824	14.035	14.448	1.00 35.05	A
	MOTA	2274	Ō	ALA	Α	357		21.194	14.561	15.369	1.00 35.04	A
	ATOM	2275	N	LEU	Α	358		22.516	14.730	13.552	1.00 37.81	A
	ATOM	2276	CA	LEU	Α	358		22.578	16.185	13.597	1.00 42.15	A
5	ATOM	2277	СВ	LEU	Α	358		23.679	16.681	12.658	1.00 39.54	A
	ATOM	2278	CG			358		25.086	16.285	13.109	1.00 39.51	A
•	ATOM	2279	CD1					26.102	16.686	12.062	1.00 39.29	A
	MOTA	2280	CD2	LEU				25.395	16.953	14.445	1.00 40.01	A
	ATOM	2281	C			358		21.241	16.837	13.242	1.00 45.91	· A
10	ATOM	2282	Ö			358		20.874	16.927	12.069	1.00 45.71	A
-	ATOM	2283	N			359		20.530	17.290	14.275	1.00 50.06	A
	ATOM	2284	CA			359		19.223	17.939	14.140	1.00 53.73	A
	ATOM	2285	CB			359		19.353	19.428	13.726	1.00 54.04	A
	ATOM	2286	OG1			359		19.995	19.521	12.448	1.00 56.35	A
15	ATOM	2287		THR				20.158	20.204	14.763	1.00 54.32	A
	ATOM	2288	C .			359		18.309	17.236	13.139	1.00 54.47	A
	ATOM	2289	ō.	THR				18.483	16.016	12.930	1.00 55.90	A
	ATOM	2290	OXT	THR				17.407	17.908	12.595	1.00 56.97	A
	ATOM	2291	OH2	TIP	S	1		42.566	19.118	34.302	1.00 15.09	S
20	ATOM	2292	OH2		S	2		41.052	32.378	19.857	1.00 15.82	s
	ATOM	2293		TIP	s	3		37.014	33.030	17.747	1.00 16.95	S
	ATOM	2294	OH2	TIP	s	5		45.353	24.370	18.152	1.00 16.85	S
	MOTA	2295	OH2	TIP	s	6		31.896	13.930	33.235	1.00 20.42	s
	ATOM	2296	OH2	TIP	s	7		50.351	22.781	28.249	1.00 21.14	s
25	MOTA	2297	OH2	TIP	s	8		45.246	-0.589	-0.734	1.00 17.74	S
	MOTA	2298	OH2	TIP	s	11		46.249	-0.348	-8.523	1.00 21.32	s
	ATOM	2299	OH2	TIP	s	14		45.756	11.148	29.680	1.00 21.94	S
	ATOM	2300	OH2	TIP	s	15		44.273	13.157	34.592	1.00 15.61	S
	ATOM	2301	OH2	TIP	S	17		53.598	3.722	-1.720	1.00 21.45	. S
30	MOTA	2302	OH2	TIP	S	18		46.049	13.087	31.565	1.00 20.35	S
	ATOM	2303	OH2	TIP	S	19		53.422	22.401	-3.280	1.00 23.26	S
	MOTA	2304	OH2	TIP	S	20		34.587	7.922	5.383	1.00 22.58	s
	ATOM	2305	OH2	TIP	S	21		45.053	27.379	19.376	1.00 29.60	S
	ATOM	2306	OH2		S	23		28.899	36.416	28.633	1.00 31.68	S
35	ATOM	2307	OH2		S	24		35.531	11.645	-8.219	1.00 23.45	S
	ATOM	2308	OH2		S	25		47.364	28.787	19.612	1.00 23.03	S
	ATOM	2309	OH2	ŢIP	S	27		48.859	21.588	12.634	1.00 23.76	S
	MOTA	2310	OH2		S	29		48.805	8.920	23.626	1.00 22.23	S
	ATOM	2311	OH2		S	31		48.619	7.247	10.112	1.00 21.32	S
40	ATOM	2312	OH2	TIP	s	34		44.824	28.720	15.621	1.00 25.27	S
	ATOM	2313	OH2		S	35		26.030	12.634	13.407	1.00 21.61	S
	ATOM	2314	OH2		S	36		50.462	19.810	40.066	1.00 25.45	S
	ATOM	2315	OH2		S	37		39.631	23.510	-0.239	1.00 30.88	S
45	ATOM	2316		TIP		40		44.734	42.655	10.346	1.00 30.84	S
45	ATOM	2317		TIP		41		54.653	3.902	1.503	1.00 27.14	S
	ATOM	2318		TIP		45		45.693	21.923	39.754	1.00 28.30	S
	ATOM	2319		TIP		47		47.820	16.413	7.805	1.00 25.73	S
	ATOM	2320		TIP		48		50.292	31.412	29.642	1.00 32.79	S
50	ATOM	2321 2322		TIP TIP		49		26.056	16.646	34.827	1.00 29.80	S
30	ATOM ATOM	2323		TIP		52 53		31.714	10.996	31.855	1.00 29.15 1.00 24.21	S
	ATOM	2323		TIP		54		46.108	23.843	-4.299		S
				TIP		55		37.645	11.206	34.448	1.00 28.56	S
	ATOM ATOM	2325 2326		TIP		58		26.371 33.564	28.513	12.142	1.00 32.08	S
55	ATOM	2320		TIP		64		48.295	19.700 -0.632	3.483 14.280	1.00 28.28 1.00 32.13	s s
<i>JJ</i>	ATOM	2328		TIP		65		40.293	26.036	34.324	1.00 32.13	s S
	ATOM	2329		TIP		66		29.570	3.958	14.729	1.00 24.17	S
	ATOM	2329		TIP		72		60.085	11.604	6.814	1.00 28.94	S
	ATOM	2331		TIP		73		39.203	44.403	18.686	1.00 36.33	S
	222.011		V112		_	, ,	•		14.400	10.000	1.00 20.UI	ن

	ATOM	2332	OH2 TIP S	76	47.312	12.366	27.366	1 00	28.51	
										S
	ATOM	2333	OH2 TIP S			33.771	33.329		28.82	S.
	ATOM	2334	OH2 TIP S		57.890	13.106	2.128	1.00	40.62	S
	ATOM	2335	OH2 TIP S	82	41.663	34.381	32.043	1.00	19.35	s
5	ATOM	2336	OH2 TIP S		50.974	40.331	19.200		21.14	S
•	ATOM	2337	OH2 TIP S							
					47.925	-0.832	-6.556		24.11	. S
	ATOM	2338	OH2 TIP S		27.231	28.336	33.481		27.64	S
	MOTA	2339	OH2 TIP S	91	43.651	-7.101	-7.995	1.00	24.33	S
	MOTA	2340	OH2 TIP S	92	49.325	4.387	19.370	1.00	28.02	s
10	ATOM	2341	OH2 TIP S	93	46.231	11.549	33.898		29.40	s
	ATOM	2342	OH2 TIP S		63.889	24.831	1.168		26.53	
										S
	ATOM	2343	OH2 TIP S		56.396	4.952	-6.749		28.00	s
	ATOM	2344	OH2 TIP S		35.510	27.986	11.558		29.24	s
	ATOM	2345	OH2 TIP S	100	49.942	24.366	30.265	1.00	31.61	S
15	ATOM	2346	OH2 TIP S	101	56.121	7.113	-8.298		31.57	S
	ATOM	2347	OH2 TIP S		58.318	19.957	-8.378		26.95	S
	ATOM	2348	OH2 TIP S		49.647	22.446	39.624		40.57	S
	MOTA	2349	OH2 TIP S		45.359	7.052	13.052		26.27	s
	ATOM	2350	OH2 TIP S	105	37.150	32.340	32.346	1.00	34.45	S
20	MOTA	2351	OH2 TIP S	107	43.465	40.457	8.240	1.00	40.48	s
	ATOM	2352	OH2 TIP S		36.644	8.257	13.418		30.70	S
	ATOM	2353		123	41.912	-8.974	-8.264			
									26.08	S
	MOTA	2354	OH2 TIP S		62.424	15.800	-7.411			s
	ATOM	2355	OH2 TIP S	126	37.266	18.656	-9.097	1.00	28.99	S
25	ATOM	2356	OH2 TIP S	127	43.129	26.845	14.606	1.00	25.19	S
	ATOM	2357	OH2 TIP S	128	36.339	32.639	29.802	1.00	29.25	S
	ATOM	2358			54.051	14.561	26.498		33.93	Š
	ATOM	2359	OH2 TIP S							
					41.805	-4.242	5.492		33.72	S
	MOTA	2360	OH2 TIP S		38.873	25.163	36.697		30.69	S
30	ATOM	2361	OH2 TIP S	134	28.777	8.553	25.307	1.00	31.43	S
	ATOM	2362	OH2 TIP S	135	53.672	10.546	-12.803	1.00	33.45	S
	ATOM	2363	OH2 TIP S	136	59.892	15.434	11.467	1.00	31.39	S
	MOTA	2364	OH2 TIP S	137	31.040	12.361	35.470		34.07	S
		2365		139						S
	ATOM				33.489	14.292	-0.598		40.68	
35	ATOM	2366	OH2 TIP S	140	46.918	8.748	11.662		29.23	S
	ATOM	2367	OH2 TIP S	141	46.297	-7.287	-9.196	1.00	42.20	S
	ATOM	2368	OH2 TIP S	142	58.193	6.715	-4.685	1.00	35.48	s.
	ATOM	2369	OH2 TIP S	143	44.598	4.435	12.503	1.00	27.68	s
	ATOM	2370	OH2 TIP S	144	27.003	5.999	12.450		36.30	S
40	ATOM	2371	OH2 TIP S	145	43.676	32.852	35.735		35.70	S
40										
	ATOM	2372	OH2 TIP S	146	35.783	18.628	36.452		34.62	S
	ATOM	2373	OH2 TIP S	147	25.402	4.058	20.638		45.03	S
	ATOM	2374	OH2 TIP S	148	45.839	35.853	33.724	1.00	35.47	s
	ATOM	2375	OH2 TIP S	149	22.176	18.976	16.752	1.00	31.87	S
45	ATOM	2376	OH2 TIP S	150	43.986	33.179		1.00	37.70	s
	ATOM	2377	OH2 TIP S		50.653		42.428		35.80	S
	ATOM	2378	OH2 TIP S		47.843	24.314	9.506		31.05	S
	ATOM	2379	OH2 TIP S		44.693		-14.175	1.00	29.90	s
	ATOM	2380	OH2 TIP S	155	26.560	36.851	31.684	1.00	49.29	s
50	ATOM	2381	OH2 TIP S	156	46.867	8.019	-12.951	1.00	29.21	S
	ATOM	2382	OH2 TIP S		30.432	28.741	12.438		37.76	s
	ATOM	2383							39.53	S
			OH2 TIP S		41.004	20.553	6.423			
	MOTA	2384	OH2 TIP S		49.258	20.069	29.294	1.00		S
	MOTA	2385	OH2 TIP S		48.082	28.459	16.489	1.00		S
55	ATOM	2386	OH2 TIP S	161	47.448	18.625	27.683	1.00	34.87	S
	ATOM	2387	OH2 TIP S		19.687	20.632	23.411	1.00		S
	ATOM	2388	OH2 TIP S		32.402	-1.266	22.443		37.26	s
								1.00		
	ATOM	2389	OH2 TIP S		39.475	33.468	33.237			S
	ATOM	2390	OH2 TIP S	T P P	44.277	18.950	5.162	1.00	45.14	S

	ATOM	2391	OH2 TIP S	3 166	34.79	7 30.523	10.736	1.00 47.55	s
	ATOM	2392	OH2 TIP S	167	46.54	1 3.526	-14.949	1.00 26.54	·s
	ATOM	2393	OH2 TIP S	168	36.33			1.00 38.68	S
	ATOM	2394		3 169 °					
					-			1.00 34.66	S
5	ATOM	2395	OH2 TIP S		24.16		11.375	1.00 41.23	S
	MOTA	2396	OH2 TIP S	3 171	48.45	9 15.018	31.951	1.00 38.11	S
	ATOM	2397	OH2 TIP S	172	34.26	1 23.193	40.004	1.00 48.96	s
	ATOM	2398		173	45.92			1.00 39.55	s
	ATOM	2399	OH2 TIP S						
10					41.38			1.00 40.74	S
10	ATOM	2400		177	49.39			1.00 44.33	, S
	ATOM	2401	OH2 TIP S	178	29.06	6 29.942	34.359	1.00 41.46	S
	MOTA	2402	OH2 TIP S	180	49.35	4 19.467	7.273	1.00 34.56	s
	ATOM	2403	OH2 TIP S	181	25.29			1.00 47.74	S
	ATOM	2404	OH2 TIP S						
1.0					37.07			1.00 43.87	S
15	ATOM	2405	OH2 TIP S		22.58		18.691	1.00 41.75	S
	ATOM	2406	OH2 TIP S	184	32.26	9 7.011	-1.891	1.00 48.84	S
	ATOM	2407	OH2 TIP S	185	48.23	4 0.494	6.833	1.00 48.16	s
	ATOM	2408	OH2 TIP S	187	20.00		19.211	1.00 45.27	s
	ATOM	2409	OH2 TIP S		49.34		42.272		S
20								1.00 42.20	
20	ATOM	2410	OH2 TIP S		61.29		-8.097	1.00 45.21	S
	ATOM	2411		191	28.15	2 10.606	2.819	1.00 40.38	S
	ATOM	2412	OH2 TIP S	192	25.62	6 12.619	23.191	1.00 34.27	S
	ATOM	2413	OH2 TIP S	193	59.87	6 11.603	1.216	1.00 46.54	S
	ATOM	2414		194	57.59		-10.646	1.00 45.82	S
25									
25	ATOM	2415	OH2 TIP S		31.50		21.499	1.00 38.73	S
	MOTA	2416	OH2 TIP S		50.27		-6.136	1.00 42.66	S
	MOTA	2417	OH2 TIP S	198	24.46	7 8.729	13.088	1.00 42.78	S
	ATOM	2418	OH2 TIP S	199	38.09	8 8.699	25.759	1.00 32.80	S
	ATOM	2419	OH2 TIP S	200	57.83		-13.255	1.00 45.31	. S
30	ATOM	2420	OH2 TIP S		23.88		30.524	1.00 37.12	S
50									
	ATOM	2421			47.69		37.666	1.00 37.92	S
	ATOM	2422	OH2 TIP S		38.65		29.307	1.00 50.54	S
	ATOM	2423	OH2 TIP S	206	44.42	4 27.583	2.092	1.00 53.50	S
	ATOM	2424	OH2 TIP S	212	22.25	8 2.296	17.948	1.00 47.38	S
35	ATOM	-2425	OH2 TIP S	214	19.84		23.303	1.00 30.36	S
	ATOM	2426	OH2 TIP S		27.64		24.681	1.00 31.32	S
									S
	ATOM	2427	OH2 TIP S		37.95		-9.284	1.00 45.97	
	MOTA	2428	OH2 TIP S		33.84		12.124	1.00 38.11	S
	ATOM	2429	OH2 TIP S	219	58.48	4 15.269	13.717	1.00 38.26	S
40	ATOM	2430	OH2 TIP S	220	48.52	6 40.920	26.583	1.00 35.23	S
	ATOM	2431	OH2 TIP S		52.09		38.122	1.00 29.86	s
	ATOM	2432	OH2 TIP S		36.88		3.281	1.00 37.63	S
	ATOM								S
		2433	OH2 TIP S		47.64		-10.684	1.00 34.89	
	MOTA	2434	OH2 TIP S	226	47.28		19.133	1.00 34.10	S
45	ATOM	2435	OH2 TIP S	227	42.46	3 4.463	-15.039	1.00 37.98	S
	ATOM	2436	OH2 TIP S	228	19.16	9 22.832	21.831	1.00 41.57	S
	ATOM	2437	OH2 TIP S		57.59			1.00 50.22	s
	ATOM	2438	OH2 TIP S		27.10		5.655	1.00 40.57	S
	ATOM	2439	OH2 TIP S		58.61		-11.925	1.00 50.71	S
50	ATOM	2440	OH2 TIP S		22.82	25.342	19.945	1.00 34.93	S
	ATOM	2441	OH2 TIP S	236	24.83	1 32.218	28.901	1.00 37.69	s
	ATOM	2442	OH2 TIP S	237	20.04	5 10.774	16.992	1.00 39.57	s
	ATOM	2443	OH2 TIP S		58.01		15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S		19.490		26.114	1.00 34.55	S
55	ATOM	2445	OH2 TIP S		61.18		7.346	1.00 39.68	S
	ATOM	2446	OH2 TIP S	241	33.680	38.342	19.389	1.00 48.93	s
	ATOM	2447	OH2 TIP S	242	51.53	31.612	10.881	1.00 55.65	S
	ATOM	2448	OH2 TIP S		25.872		30.404	1.00 46.69	S
	ATOM	2449	OH2 TIP S				9.544	1.00 43.81	S
_	M 1 OF	2443	OUS IIE 2	240	37.332	5.849	9.344	1.00 43.01	3

	ATOM	2450	OH2 TI	9 9 250		39.087	-1.293	-9.655	1.00 42.96	i s
	•									
	ATOM	2451	OH2 TI	S 258		23.938	30.000	30.010	1.00 38.89) ; S
	ATOM	2452	OH2 TI	S 259		24.949	29.749	32.578	1.00 40.17	S
		2453	OH2 TI	-		32.111	17.986	1.918		
	MOTA								1.00 48.36	
5	ATOM	2454	OH2 TI	? S 266		21.404	12.876	25.603	1.00 57.17	'S
	ATOM	2455	OH2 TI	9 9 269		35.425	36.767	12.550	1.00 30.70	
	ATOM	2456	OH2 TIE	? S 270		52.438	25.529	30.131	1.00 44.85	S
	MOTA	2457	OH2 TIE	s 271		53.299	20.156	36.003	1.00 37.15	s s
			_			50.914	6.919	23.723		
	MOTA	2458	OH2 TI						1.00 43.29	
10	ATOM	2459	OH2 TIE	S 274		31.578	30.795	11.014	1.00 50.15	i s
	ATOM	2460	OH2 TI	9 9 275		26.341	7.243	22.447	1.00 39.40) S
٠.	•									
	MOTA	2461	OH2 TIE			60.392	18.195	10.235	1.00 37.91	
	ATOM	2462	OH2 TIP	S 277		47.355	-9.081	-10.821	1.00 48.18	S
	ATOM	2463	OH2 TIE			41.304	6 175	-16.647	1.00 38.12	
15	MOTA	2464	OH2 TIE	? S 282		33.299	21.620	37.881	1.00 46.29	S
	MOTA	2465	OH2 TIE	s 283		56.469	26.112	-8.575	1.00 43.71	. S
	ATOM	2466	OH2 TIE			48.382	26.573	7.246	1.00 41.43	
	ATOM	2467	OH2 TIE	S 288		56.240	7.245	-11.331	1.00 41.79	S
	ATOM	2468		S 290		49.060	14.978	28.166	1.00 37.03	
20	MOTA	2469	OH2 TIE	? S 291		37.095	44.270	26.442	1.00 45.08	
	ATOM	2470	OH2 TIE	S 292		47.814	-0.384	-13.299	1.00 48.60	S
								-7.841	1.00 41.89	
	MOTA	2471		S 297		58.081	2.784			
	ATOM	2472	OH2 TIE	S 298		36.447	45.321	18.644	1.00 54.91	. S
	ATOM	2473	OH2 TIE	2 2 2 9		49.029	23.328	1.767	1.00 30.55	S
25	MOTA	2474	OH2 TIE	? s 301		24.375	13.771	8.634	1.00 48.47	
	MOTA	2475	OH2 TIE	S 303		47.904	36.798	28.653	1.00 35.76	s s
			OH2 TIE			51.156	40.821	27.172	1.00 43.59	
•	ATOM	2476								
	ATOM	2477	OH2 TI	? S 306		32.943	28.917	35.227	1.00 42.60	
	MOTA	2478	OH2 TIE	2 3 307		58.462	28.373	6.251	1.00 46.15	S
20								36.712	1.00 48.26	
30	ATOM	2479	OH2 TIE	2 8 308		41.964	30.940			
	ATOM	2480	OH2 TIE	s 313		51.176	-1.922	-3.336	1.00 50.61	S
	ATOM	2481	OH2 TI	21001		21.319	36.868	23.805	1.00 36.97	s
	ATOM	2482	OH2 TIE	2 \$1002		48.880	32.620	27.617	1.00 44.40	
	ATOM	2483	OH2 TI	S1003		61.880	19.473	11.767	1.00 45.49	S
25			OH2 TI			52.770	21.424	26.815	1.00 24.43	S
35	ATOM	2484								
	MOTA	2485	OH2 TIE	? S1005		35.373	29.094	36.197	1.00 35.97	
	MOTA	2486	OH2 TI	2 S1006		40.815	-6.636	4.389	1.00 43.15	i S
							1.286	11.272	1.00 49.45	
	MOTA	2487	OH2 TI	5 21007		44.953				
	MOTA	2488	OH2 TIL	? \$1010		21.004	16.168	27.009	1.00 48.51	
40	ATOM	2489	OH2 TI	S1011		47.094	41.786	9.243	1.00 50.10	s S
40									1.00 49.47	
	ATOM	2490	OH2 TI	5 21012		32.479	2.978	14.158		
	ATOM	2491	012 GL	CG 1		48.557	11.372	-12.279	1.00 40.72	: G
	ATOM	2492	C11 GLO	C G - 1		48.836	12,133	-11.097	1.00 38.05	i G
								-11.476	1.00 38.09	
	ATOM	2493	C13 GL			49.266				
45	MOTA	2494	014 GL	CG 1		49.559	14.299	-10.292	1.00 33.99) G
			C15 GL			48.150		-12.257	1.00 37.32	
	MOTA	2495								
	ATOM	2496	016 GL	CG 1	•	48.574	15.582	-12.604	1.00 36.74	
	MOTA	2497	012 GL	C G 2		40.114	-6.634	-6.562	1.00 33.52	: G
								-7.404	1.00 31.05	
	MOTA	2498	C11 GL				-6.592			
50	ATOM .	2499	C13 GLC	CG 2		37.712	-6.417	-6.552	1.00 31.56	
	MOTA	2500	014 GL			36.554	-6.406	-7.389	1.00 30.70) G
	ATOM	2501	C15 GL			37.792	-5.109	-5.761	1.00 30.03	
	ATOM	2502	016 GL	CG 2		36.609	-4.961	-4.975	1.00 29.66	G G
			012 GL			44.030		-13.470	1.00 37.90	
	MOTA	2503								
55	MOTA	2504	C11 GL	CG 3		43.950		-13.690	1.00 38.47	
	ATOM	2505	C13 GL	C G 3		42.747	9.974	-14.579	1.00 39.52	: G
								-13.942	1.00 39.39	
	ATOM	2506	014 GL			41.551				
	ATOM	2507.	C15 GL0	CG 3		42.878	9.280	-15.934	1.00 41.43	
	ATOM	2508	016 GL			41.736	9,613	-16.731	1.00 40.78	G
	111 011	2500	210 010				5.020			

						•							
	ATOM	2509	012	GLC (3	5		40.556	1.005	2.289	1.00	45.25	G
	ATOM	2510	C11 (5		40.966	2.332	1.960	1.00	40.56	G
	ATOM	2511	C13 (5		40.187	3.327	2.814	1.00	40.36	G
	ATOM	2512	014			5		38,791	3.169	2.572	1.00	40.71	G
5	ATOM	2513	C15			5		40.619	4.751	2.464	1.00	40.04	G
3		2514	016			5		39.885	5.681	3.256	1.00	36.89	G
	ATOM		012			6		36.951	22.702	40.046	1.00	63.04	G
	MOTA	2515				6	•	37.592	21.583	39.422		62.46	G
	MOTA	2516	C11 (38.104	21.978	38.030		61.14	G
	ATOM	2517	C13 (6		39.034	23.054	38.168		61.72	, G .
10	ATOM	2518	014			6		36.948	22.429	37.126		60.51	G
•	ATOM	2519	C15 (6			21.372	36.960		58.61	Ğ
	ATOM	2520	016			6		35.992	0.281	14.299		73.45	Ğ
	MOTA	2521	012			7		37.316	-0.758	15.222		72.78	Ğ
	MOTA	2522	C11 (7		37.655	•			72.78	Ğ
15	MOTA	2523	C13 (7		36.592	-1.856	15.157		73.88	G
	ATOM	2524	014			7	•	35.320	-1.299	15:498			G
	ATOM	2525	C15			7		36.924	-2.989	16.134		73.66	G
	ATOM	2526	016			7		36.972	-2.493	17.478		75.38	G
	MOTA	2527	012	GLC	G	8		51.921	21.898	5.908		62.51	
20	ATOM	2528	C11	GLC	G	8		52.447	20.871	5.063		63.42	G
	ATOM	2529	C13	GLC	G	8		51.476	20.597	3.908		64.28	G
	ATOM	2530	014	GLC	G	8		51.297	21.794	3.150		66.28	G
	ATOM	2531	C15			8		50.121	20.137			64.49	G
	MOTA	2532	016			8		49.233	19.886	3.357		64.01	G
25	ATOM	2533	012			10		36.044	37.499	29.523		56.89	G
23	ATOM	2534	C11			10		35.164	36.645	30.259		56.97	G
	ATOM	2535	C13			10		33.849	36.489	29.494		56.11	G
		2536	014			10		33.248	37.772	.29.308		56.44	G
	ATOM	2537		GLC		10		32.900	35.580	30.277		55.84	G
20	MOTA	2538		GLC		10		31.674	35.442	29.557~	. 1.00	55.39	G
30	MOTA	2539		ATP		1		46.280	25.658	5.170		51.49	N
	ATOM			ATP		î		46.464	25.053	3.691	1.00	52.22	N
	MOTA	2540		ATP		1		47.406	23.911	3.763	1.00	51.41	N
	MOTA	2541	01G		N	1		46.794	26.182	2.784	1.00	52.07	N
	ATOM	2542				1		44.976	24.513	3.344	1.00	51.01	N
35	MOTA	2543		ATP		1		44.560	22.969	3.605		50.20	N
	MOTA	2544	PB		N	1		43.083	22.898	3.669		49.41	N
	ATOM	2545		ATP		1		45.345	22.474	4.766	1.00	50.34	N
	MOTA	2546		ATP				45.070	22.231	2.255		47.77	И
	MOTA	2547		ATP		1		45.075	20.613	2.121		42.84	N
40	MOTA	2548	PA	ATP		1		45.547	20.291	0.754		43.81	N
	ATOM	2549		ATP		1		45.807	20.035	3.270		45.03	N
	MOTA	2550		ATP		1		43.516	20.223	2.245		41.73	N
	ATOM	2551		ATP		1		42.528	20.225	1.489		37.57	N
	MOTA	2552		ATP		1			20.323	1.776		39.45	N
45	ATOM	2553		ATP		1		41.127	19.024	1.279	1 00	37.72	N
	MOTA	2554		ATP		1		40.907	20.321	3.251	1 00	38.48	N
	ATOM	2555		ATP		1		40.777		3.697		40.42	N
	ATOM	2556		ATP		1		40.360	21.615			37.58	N
	MOTA	2557	C2*	ATP	N	1		39.608	19.374	3.270		35.98	N
50 -	ATOM	2558	02*	ATP	N	1		38.410	20.076	2.924		35.55	N
	MOTA	2559	C1*	ATP	N	1		39.939	18.346	2.173		31.76	N
	ATOM	2560	N9	ATP	N	1		40.628	17.156			30.49	N
	ATOM	2561	C8	ATP	N	1		41.864	17.126				
	MOTA	2562	N7	ATP		1		42.143	15.877			29.75	N N
55	ATOM	2563	C5	ATP		1		41.088	15.118			0 27.49	N N
	ATOM	2564	C4	ATP		1		40.125	15.925			0 30.02	N
	ATOM	2565		ATP		1		38.937	15.389			0 27.11	N
	ATOM	2566		ATP		1		38.679	14.085			0 25.62	N
	ATOM	2567		ATP		1		39.597	13.283	3.175	1.0	0 21.76	N
	111 011												

	ATOM	2568	С6	ATP 1	N	1	40.800	13.768	3.571		23.90	N
	ATOM	2569	N6	ATP I	N	· 1	41.698	12.964	4.127		21.94	Ŋ
	ATOM	2570	S	SO4	I	1	58.680	8.493	-0.639		56.05	I
	ATOM	2571	01		I	1	57.956	7.875	0.483		58.83	I
_		2572	02	504		1	57.886	9.607	-1.188		57.04	I
5	MOTA	2572	03		I	1	58.906	7.478	-1.683	1.00	57.47	I
	ATOM	2574	04		I	1	59.976	9.008	-0.156	1.00	57.51	I
	ATOM	2575	S		Ī	2	39.339	4.855	7.057	1.00	84.24	I
	ATOM	2575 2576	01		Ī	2	39.390	6.175	7.711		85.02	I
	MOTA	2577	02		Ī	2	40.101	4.897	5.797	1.00	84.75	I
10	MOTA		03		Ī	2	37.936	4.506	6.766	1.00	84.94	I
	MOTA	2578	04		Ì	2	39.931	3.842	7.954	1.00	84.44	I
	MOTA	2579	S		Ī	3	38.987	-2.256	3.310	1.00		I
	ATOM	2580	01			3	37.734	-1.675	3.827	1.00		I
	MOTA	2581	02			3	39.460	-1.454	2.172	1.00	59.91	I
15	MOTA	2582	02		I	3	38.743	-3.640	2.866	1.00		I
	MOTA	2583			I	3	40.014	-2.260	4.369	1.00	59.58	I
	ATOM	2584	04		I	4	34.397	5.289	30.981	1.00		I
	MOTA	2585	S	SO4	I	4	33.627	6.528	30.742	1.00	60.43	I
	MOTA	2586	01	SO4	I	4	34.337	4.427	29.782	1.00	60.11	I
20	MOTA	2587	02	SO4	I	4	33.816	4.572	32.133	1.00	64.39	I
•	MOTA	2588	03	SO4	I	4	35.806	5.626	31.277	1.00	63.55	I
	ATOM	2589	04	SO4	I	5	55.074	-6.984	-3.711	1.00	75.40	I
	MOTA	2590	S	SO4	I	5	54.657	-7.518	-2.399	1.00	74.66	I
	MOTA	2591	01		I	5	54.209	-5.845	-4.065	1.00	74.96	I
25	MOTA	2592	02	SO4		5	54.950	-8.034	-4.742	1.00	74.22	I
	MOTA	2593	03	SO4		5	56.477	-6.532	-3.633	1.00	75.15	I
	MOTA	2594	04	SO4		100	57.362	24.998	13.149	1.00	66.76	P
	MOTA	2595	02	PO4		100	59.399	26.166	13.761	1.00	66.89	P
	MOTA	2596	03	PO4		100	57.761	25.606	15.462	1.00	67.43	P
30	MOTA	2597	04	PO4			57.264	27.325	13.818	1.00	65.91	P
	MOTA	2598	01	PO4		100	57.947	26.025	14.048	1.00	66.69	P
	MOTA	2599	P	PO4	P	100	31.541	20.000				
	END											

Example 4: Co-ordinates for the dimer of the PDK1 fragment, without alternate side chains. Chain A is the molecule for which co-ordinates are given in Examples 2 and 3, and chain B is the symmetry-related molecule.

40 45 50	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	1 2 3 4 5 6 7 8 9 10 11 12 13 14	CB CG CO N CD CA N CD CA CB CG C	PRO A	71 71 71 71 71 71 72 72 72 72 72 72 72	58.912 59.621 59.493 59.196 60.984 60.554 60.040 59.356 59.712 58.840 58.672 59.796 57.527 56.710	-7.251 -6.941 -6.506 -5.318 -6.073 -5.762 -7.035 -7.385 -8.816 -6.986 -8.321 -9.133 -6.208 -6.451 -5.268 -4.454	8.216 9.534 5.894 5.766 7.833 9.207 7.217 4.890 4.898 3.578 2.858 3.419 3.673 4.561 2.753 2.708	1.00 67.78 1.00 69.16 1.00 67.06 1.00 66.66 1.00 67.86 1.00 67.75 1.00 66.32 1.00 67.17 1.00 65.61 1.00 66.47 1.00 67.57 1.00 63.94 1.00 64.11 1.00 61.57 1.00 58.74	A A A A A A A A A A A A A A A
	ATOM	16	CA	ALA A	73	56.133 56.438	-4.454 -3.030	2.708 3.165	1.00 58.74	A
55	MOTA	17	CB	ALA A	73	50,430	3.050			

		-										
•	АТОМ	18	С	ALA A	73		55.626	-4.448	1.271	1.00 5		A
	ATOM	19	0	ALA Á	73		56.347	-4.834	0.349	1.00 5		A
	ATOM	20	N	PRO A	74		54.372	-4.024	1.057	1.00 5		Α
	MOTA	21	CD	PRO A	74		53.335	-3.610	2.018	1.00 5		A
5	ATOM	22	CA	PRO A	74		53.856	-4.003	-0.314	1.00 5		. A
	ATOM	23	CB	PRO A	74		52.474	-3.375	-0.148	1.00 5		A
	ATOM	24	CG	PRO A	74		52.067	-3.824	1.226	1.00 5		A
	ATOM	25	С	PRO A	74		54.772	-3.167	-1.204	1.00 5		Α.
	ATOM	26	0	PRO A	74		55.559	-2.361	-0.708	1.00 4		A
10	ATOM	27	N	ALA A	75		54.680	-3.366	-2.514	1.00 4		A
	ATOM	28	CA	ALA A	75		55.503	-2.602	-3.446		44.69	A
	ATOM	29	CB	ALA A	75		55.312	-3.121	-4.870		46.14	A
	ATOM	30	С	ALA A	75		55.100	-1.134	-3.371		41.55	A
	MOTA	31	0	ALA A	75		53.947	-0.813	-3.086		41.01	A
15	ATOM	32	N	LYS A	76		56.053	-0.245	-3.619		38.31	A
	ATOM	33	CA	LYS A	76		55.781	1.184	-3.588	1.00		A
	ATOM	34	CB	LYS A	76		57.053	1.957	-3.930	1.00		A
	ATOM	35	CG	LYS A	76		57.123	3.356	-3.350	1.00		A
	ATOM	36	CD	LYS A	76		57.262	3.316	-1.836	1.00		A
20	MOTA	37	CE	LYS A	76		57.511	4.705	-1.277		42.08	A
	ATOM	38	NZ	LYS A	76		57.681	4.695	0.202	1.00		A
	ATOM	39	С	LYS A	76		54.708	1.467	-4.638	1.00		A
	ATOM	40	0	LYS A	76		54.814	1.005	-5.770	1.00		A.
	ATOM	41	N	LYS A	. 77		53.668	2.207	-4.270	1.00		A
25	ATOM	42	CA	LYS A	. 77		52.619	2.517	-5.232		25.72	A
	ATOM	43	CB	LYS A	. 77		51.316	2.865	-4.509	1.00		A
	ATOM	44	CG	LYS A	. 77		50.796	1.731	-3.631		27.15	A
	MOTA	45	CD	LYS A	. 77		49.487	2.089	-2.967		26.80	A
	ATOM	46	CE	LYS A	. 77		49.136	1.091	-1.870	1.00		A A
30	MOTA	47	ΝZ	LYS A	. 77		48.998	-0.296	-2.380		27.17	A
	ATOM	48	С	LYS A	. 77		53.053	3.668	-6.137		24.67	A
	MOTA	49	0	LYS A			54.010	4.377	-5.829		21.60 23.66	A
	MOTA	50	N	ARG A	78		52.351	3.838	-7.254		26.14	A
	MOTA	51	CA	ARG A			52.662	4.897	-8.211		28.57	A
35	MOTA	52	CB	ARG A			53.574	4.344	-9.318		34.78	A
	MOTA	53	CG	ARG A		,	53.017		-10.050		40.96	A
	ATOM	54	CD	ARG A		,	54.092	2.465	-10.896		48.93	A
	MOTA	55	NE	ARG A			53.560		-11.700		52.58	A
-	ATOM	56	cz	ARG A			52.985		-11.203 -9.889		54.60	A
40	MOTA	57		l ARG F			52.860	0.113	-12.022		54.09	A
	MOTA	58		2 ARG F			52.530		-8.803		23.76	A
	MOTA	59	С	ARG F			51.382 50.311	5.488 4.888	-8.706		24.25	A,
	ATOM	60	0	ARG A			<u>=</u>	6.676	-9.428		21.76	A
	ATOM	61	N	PRO A			51.475		-9.668		20.82	A
45	MOTA	- 62	ÇD	PRO F			52.691	7.475	-10.021	1 00	21.96	A
	MOTA	63	CA	PRO F			50.301	0 401	-10.816	1 00	22.27	A
	ATOM	64	CB	PRO F			50.910	0.401	-10.014		22.12	A
	MOTA	65	CG	PRO A			52.124		-10.903		22.86	A
	MOTA	66	С	PRO A			49.446	6.413	-10.842		20.52	A
50	MOTA	67	0	PRO A			48.213		-11.714		21.87	A
	ATOM	68	N	GLU A			50.103	J. 500	-12.628		22.99	A
	MOTA	69	CA				49.403	3 004	-13.571		25.24	A
	ATOM	70	CB	GLU A			50.393	J. JJ4 2 QA7	-12.925	1.00	28.75	A
	MOTA	71	CG				51.230 52.157	2.307	-13.913		31.99	A
55	ATOM	72	CD					2.224	-14.433		34.34	A
	ATOM	73		1 GLU A			53.072	2.03/ 1 N1E	-14.172		32.83	A
	ATOM	74		2 GLU A			51.969		-11.912	1.00	22.09	A
	MOTA	75	С	GLU A			48.556		-12.530	1.00	22.37	A
	MOTA	76	0	GLU A	80		47.692	3.013	-12.330			_

	MOTA	77	N	ASP A	81	48.804	3.413 -10.622	1.00 19.97	A
	ATOM	78	CA	ASP A	81	48.026	2.423 -9.874	1.00 19.93	A
	ATOM	79	CB	ASP A	81	48.736	2.029 -8.571	1.00 21.19	A
	ATOM	80	CG	ASP A	81	50.089	1.380 -8.807	1.00 22.46	A
5	ATOM	81	OD1	ASP A	81	50.195	0.554 -9.731	1.00 24.22	Α
•	· ATOM	82		ASP A	81	51.043	1.685 -8.058	1.00 23.33	A
	ATOM	83	C	ASP A	81	46.652	2.975 -9.518	1.00 20.85	A
	ATOM	84	ō	ASP A	81	45.793	2.246 -9.015	1.00 19.96	A
	ATOM	85	N	PHE A	82	46.445	4.258 -9.804	1.00 18.91	A
10	ATOM	86	CA	PHE A	82	45.200	4.934 -9.465	1.00 19.30	A
10	ATOM	87	СВ	PHE A	82	45.475	6.027 -8.427	1.00 18.43	A
-	ATOM	88	CG -		82	46.134	.5.531 -7.175	1.00 18.01	A
	ATOM	89		PHE A	82	45.371	5.136 -6.084	1.00 17.19	A
	ATOM	90		PHE A	82	47.520	5.460 -7.086	1.00 18.99	A
15	ATOM	91	-	PHE A	82	45.977	4.676 -4.918	1.00 17.12	A
13	ATOM	92		PHE A	82	48.137	5.000 -5.925	1.00 19.64	· А
	ATOM	93	CZ	PHE A	82	47.361	4.607 -4.838	1.00 18.00	A
	ATOM	94	C	PHE A		44.476	5.596 -10.621	1.00 20.81	A
		95	0	PHE A	82	45.066	5.933 -11.649	1.00 20.34	Α
20	MOTA	95 96	Ŋ	LYS A		43.182	5.792 -10.411	1.00 19.80	Α
20	MOTA	96 97	CA	LYS A		42.321	6.478 -11.353	1.00 21.65	A
	MOTA		CB	LYS A		41.096	5.625 -11.687	1.00 22.02	À
	ATOM	98 99	CG	LYS A		40.062	6.326 -12.550	1.00 28.93	. A
	ATOM			LYS A		38.974	5.355 -12.981	1.00 34.20	Α
0.5	ATOM	100	CD	LYS. A		37.909	6.042 -13.824	1.00 38.10	A
25	ATOM	101	CE	LYS A		37.179	7.086 -13.043	1.00 43.33	Α
	ATOM	102	NZ	LYS A		41.913	7.702 -10.541	1.00 20.74	Α
	MOTA	103	. C	LYS A		41.084	7.606 -9.635	1.00 20.98	A
	ATOM	104	O N	PHE A		42.513	8.848 -10.835	1.00 19.99	A
20	MOTA	105	CA	PHE A		42.188	10.049 -10.083	1.00 18.63	A
30	MOTA	106 107	CB	PHE A		43.279	11:103 -10.258	1.00 18.95	A
	ATOM	108	CG	PHE A		44.571	10.741 -9.587	1.00 17.68	A
	ATOM ATOM	100		PHE A		45.498	9.926 -10.224	1.00 18.16	Α
	ATOM	110		PHE A		44.843		1.00 19.66	A
35	ATOM	111		PHE A		46.676	9.556 -9.589	1.00 18.09	A
33	ATOM	112		PHE A		46.021	10.816 -7.653	1.00 18.89	A
	ATOM	113	CZ	PHE A		46.936	10.002 -8.301	1.00 17.33	A
	ATOM	114	C	PHE A		40.834	10.617 -10.460	1.00 19.69	A
	ATOM	115	o	PHE A		40.391	10.489 -11.601	1.00 20.72	Α
40	ATOM	116	N	GLY A		40.178	11.233 -9.484	1.00 16.80	Α
40	ATOM	117	CA	GLY A		38.872	11.810 -9.716	1.00 17.73	Α
	MOTA	118	C	GLY A		38.819	13.280 -9.346	1.00 18.75	. A
	ATOM	119	Ö	GLY A		39.740	14.043 -9.650	1.00 18.45	A
	ATOM	120	N	LYS A		37.753	13.673 -8.659	1.00 16.00	A
45	ATOM	121	CA	LYS A		37.571	15.064 -8.278	1.00 18.26	A
43	ATOM	122	CB	LYS A		36.133	15.302 -7.812	1.00 19.00	Α
	ATOM	123	CG	LYS A		35.793	14.660 -6.481	1.00 21.55	A
	ATOM	124	CD	LYS A		34.368	14.981 -6.066	1.00 26.48	A
	ATOM	125	CE	LYS A		33.994	14.239 -4.793	1.00 31.92	Α
50	ATOM	126	NZ	LYS A		32.568	14.457 -4.412	1.00 35.36	A
- 50	ATOM	127	C	LYS A		38.523	15.571 -7.202	1.00 18.57	Α
	ATOM	128	Ö	LYS A		39.045	14.807 -6.385	1.00 16.77	Α
	MOTA	129	N	ILE A		38.737	16.881 -7.227	1.00 17.88	Α
	ATOM	130	CA	ILE A		39.577	17.554 -6.256	1.00 18.26	A
55	MOTA	131	CB	ILE P		39.994	18.952 -6.772	1.00 19.60	A
,,	ATOM	132	CG2		-	40.593	19.786 -5.628	1.00 18.73	A
	ATOM	133		L ILE A			18.786 -7.945	1.00 21.16	A
	ATOM	134		L ILE P			20.087 -8.588	1.00 25.26	A
	ATOM	135	C C J	ILE P			17.709 -4.997	1.00 19.67	A
	211 011	100	-		- 0.				

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	ATOM	136	0	ILE	A	87	37.628	18.249	-5.052	1.00 20.41	A
	ATOM	137	N	LEU		88	39.240	17.229	-3.867	1.00 19.15	Α
	ATOM '	138	CA	LEU	A	88	38.508	17.324	-2.611	1.00 20.68	A
	MOTA	139	CB	LEU		88	38.870	16.151	-1.700	1.00 19.97	А
5	ATOM	140	CG	LEU		88	38.529	14.759	-2.237	1.00 19.24	. A
	ATOM	141	CD1	LEU	A	88	39.090	13.692	-1.311	1.00 21.41	A
	ATOM	142	CD2	LEU	A	88	37.029	14.622	-2.359	1.00 18.84	A
	ATOM	143	С	LEU	Α	88	38.815	18.632	-1.901	1.00 23.11	A
	ATOM	144	0	LEU	Α	88	37.999	19.146	-1.139	1.00 25.10	A
10	ATOM	145	N	\mathtt{GLY}		89	39.997	19.174	-2.149	1.00 24.09	A
	MOTA	146	CA	GLY	Α	89	40.367	20.418	-1.507	1.00 24.27	A
	ATOM	147	С	GLY	Α	89	41.658	20.954	-2.078	1.00 25.47	A
	MOTA	148	0	GLY	Α	89	42.445	20.202	-2.666	1.00 22.19	A
	MOTA	149	N	GLU	Α	90	41.870	22.254	-1.906	1.00 26.22	A
15	MOTA	150	CA	GLU	Α	90	43.064	22.924	-2.404	1.00 29.96	Α
	ATOM	151	СВ	GLU	Α	90	42.698	23.814	-3.596	1.00 30.75	A
	ATOM	152	CG	GLU	Α	90	42.267	23.038	-4.831	1.00 34.32	A
	MOTA	153	CD	GLU	Α	90	41.711	23.930	-5.927	1.00 38.27	A
	ATOM	154	OE1	GLU	Α	90 .	40.590	24.456	-5.764	1.00 40.57	A
20	MOTA	155	OE2	GLU	Α	90	42.398	24.110	-6.952	1.00 40.90	A
	MOTA	156	С	GLU	Α	90	43.711	23.768	-1.313	1.00 30.68	A
	ATOM	157	0	GLU	Α	90	43.049	24.574	-0.668	1.00 32.83	A
	MOTA	158	N	GLY	Α	91	45.006	23.566	-1.104	1.00 29.66	A
	ATOM	159	CA	GLY	Α	91	45.724	24.332	-0.104	1.00 29.40	A
25	ATOM	160	С	GLY	Α	91	46.795	25.151	-0.798	1.00 29.98	A
	ATOM	161	0	GLY	Α	91	46.894	25.130	-2.028	1.00 28.16	Α
	MOTA	162	N	SER	Α	92	47.605	25.870	÷0.029	1.00 28.30	A
	ATOM	163	CA	SER	Α	92	48.653	26.681	-0.633	1.00 30.50	A
	ATOM	164	CB	SER	A	92	49.165	27.717	0.370	1.00 32.43	A
30	ATOM	165	OG	SER	Α	92	49.520	27.099	1.593	1.00 40.94	A
	ATOM	166	С	SER	Α	92	49.815	25.843	-1.164	1.00 29.77	Α
	ATOM	167	0	SER	Α	92	50.456	26.221	-2.143	1.00 30.46	А
	ATOM	168	N	PHE	Α	93	50.087	24.703	-0.536	1.00 27.65	A
	ATOM	169	CA	PHE	Α	93	51.185	23.855	-0.995	1.00 26.34	A
35	ATOM	170	CB	PHE	Α	93	52.281	23.785	0.068	1.00 27.95	A
	ATOM	171	CG	PHE	Α	93	52.861	25.117	0.406	1.00 31.06	A
	ATOM	172	CD1	PHE	Α	93	52.283	25.909	1.392	1.00 29.96	A
	ATOM	173	CD2	PHE	Α	93	53.949	25.613	-0.308	1.00 31.38	А
	ATOM	174			Α	93	52.779	27.181	1.665	1.00 32.69	A
40	ATOM	175	CE2	PHE	Α	93	54.452	26.883	-0.044	1.00 32.63	A
	ATOM	176	CZ	PHE	A	93	53.864	27.670	0.945	1.00 31.81	A
	ATOM	177	С	PHE	Α	93	50.759	22.445	-1.365	1.00 25.39	A
	ATOM	178	0	PHE	Α	93	51.601	21.559	-1.522	1.00 24.59	Α
	MOTA	179	N	SER		94	49.457	22.235	-1.519	1.00 23.63	Α
45	ATOM	180	CA	SER	Α	94	48.965	20.912	-1.860	1.00 21.43	A
	MOTA	181	CB	SER	Α	94	49.017	20.013	-0.628	1.00 21.42	Α
	ATOM	182	OG	SER	A	94	48.091	20.475	0.340	1.00 21.19	A
	MOTA	183	С	SER	A	94	47.539	20.925	-2.378	1.00 19.82	Α
	MOTA	184	0	SER	Α	94	46.795	21.882	-2.173	1.00 18.76	Α
50	ATOM	185	N	THR		95	47.174	19.832	-3.038	1.00 19.38	Α
	ATOM	186	CA	THR	A	95	45.840	19.637	-3.580	1.00 17.98	A
	ATOM	187	CB	THR		95	45.818	19.818	-5.110	1.00 19.25	A
	ATOM	188		THR		95	46.196	21.162	-5.434	1.00 22.04	A
	ATOM	189		THR		95	44.421	19.549	-5.661	1.00 17.61	A
55	ATOM	190	С	THR		95	45.455	18.201	-3.243	1.00 18.61	A
	ATOM	191	O٠	THR		95.	46.212	17.264	-3.524	1.00 17.10	A
	ATOM	192	N	VAL		96	44.295	18.024	-2.623	1.00 16.53	Α
	ATOM	193	CA	VAL		96	43.845	16.685	-2.266	1.00 16.05	A
	ATOM	194	CB	VAL	A	96	43.170	16.672	-0.886	1.00 16.32	A

	ATOM	195	CG1	VAL	Α	96		42.74	1	15.249	-0.532	1.00	18.02	Α
	ATOM	196	CG2	VAL	Α	96		44.14	5	17.206	0.168	1.00	16.69	A
	MOTA	197	С	VAL		96		42.87	5	16.207	-3.335	1.00	16.42	A
	MOTA	198	0	VAL		96		41.90	6	16.892	-3.665		16.47	A
5	ATOM	199	N	VAL		97		43.15		15.033	-3.888		16.80	A
,	ATOM	200	CA	VAL		97		42.338		14.471	-4.949		16.72	A
		201	CB	VAL		97		43.153		14.354	-6.255		18.43	A
	ATOM							42.249		13.927	-7.404			
	ATOM	202		VAL		97							19.69	A
	MOTA	203		VAL		97		43.83		15.685	-6.569		17.84	A
10	ATOM	204	C	VAL		97		41.812		13.091	-4.583		16.77	A
	MOTA	205	0	VAL		97		42.532		12.270	-4.014		17.13	A
	ATOM	206	N	LEU		98		40.54		12.845	-4.895		16.62	A
	ATOM	207	CA	LEU		98		39.94		11.548	-4.624		17.04	A
	MOTA	208	CB	LEU	Α	98		38.42	4	11.633	-4.743		16.89	A
15	ATOM	209	CG	LEU	Α	98		37.63	5	10.342	-4.508	1.00	19.46	А
	MOTA	210	CD1	LEU	A	98		37.990	0	9.762	-3.146	1.00	20.07	Α
	ATOM	211	CD2	LEU	Α	98		36.143	3	10.627	-4.588	1.00	17.93	Α
	ATOM	212	С	LEU	Α	98		40.512	2	10.597	-5.677	1.00	17.38	A
	ATOM ·	213	0	LEU	Α	98		40.52	7	10.920	-6.863	1.00	18.60	A
20	ATOM	214	N	ALA		99	-	40.99	5	9.438	-5.246	1.00	17.13	A
	ATOM	215	CA	ALA		99		41.570	0	8.466	-6:168	1.00	18.42	Α
	ATOM	216	CB	ALA		99	•	43.090		8.524	-6.105		14.76	Α
	ATOM	217	C	ALA		99		41.102		7.055	-5.848		21.40	A
	ATOM	218	Ö	ALA		99		40.94		6.691	-4.679		22.52	A
25		219	N	ARG				40.878		6.261	-6.888		19.77	A
23	ATOM			ARG				40.45		4.884	-6.693		20.85	A
	ATOM	220	CA					39.20		4.585	-7.518		24.22	A
	ATOM	221	CB	ARG				38.60		3.205	-7.256		31.78	A
	MOTA	222	CG	ARG									36.24	A
	MOTA	223	CD	ARG				37.32		2.979	-8.048			A
30	ATOM	224	NE	ARG				36.213		3.818	-7.594		41.40	
	MOTA	225	CZ	ARG				35.56		3.662	-6.439		42.05	A
	MOTA	226		ARG				35.91		2.696	-5.598		40.67	A
	MOTA	227		ARG				34.55		4.468	-6.128		43.65	A
	ATOM	228	С	ARG				41.61		3.985	-7.129		18.63	A
35 ·	MOTA	229	0	ARG	Α	100		42.07		4.065	-8.271		19.49	A
	MOTA	230	N	GLU	Α	101		42.10		3.157	-6.212		16.43	A
	ATOM	231	CA	GLU	Α	101		43.19		2.246	-6.533		16.11	A
	ATOM	232	CB	GLU	Α	101		43.77	4	1.637	-5.248		16.79	A
	ATOM	233	CG	GLU	Α	101		44.91	7	0.657	-5.488		16.51	A
40	ATOM	234	CD	GLU	Α	101		45.50	1	0.115	-4.200	1.00	18.20	A
	ATOM	235	OE1	GLU	Α	101		44.73	3	-0.081	-3.239	1.00	18.32	A
	ATOM	236	OE2	GLU	Α	101		46.72	5	-0.132	-4.150	1.00	17.14	A
	ATOM	237	С	GLU	Α	101		42.62	5	1.152	-7.442	1.00	17.92	Α
	ATOM	238	0	GLU	Α	101		41.68	1	0.462	-7.069	1.00	18.02	A
45	ATOM	239	N	LEU	Α	102		43.19	8 .	1.002	-8.632	1.00	19.06	Α
	ATOM	240	CA	LEU				42.71		0.025	-9.607		20.71	A
	ATOM	241	СВ			102		43.56			-10.878		23.42	. A
	ATOM	242	CG	LEU				43.53			-11.642		25.30	· A
	ATOM	· 243		LEU				44.57	7	1.414	-12.748		27.88	Α
50	ATOM	244		LEU				42.14			-12.214		26.79	· А
50			C			102		42.67		-1.418	-9.125		21.62	Α
	ATOM	245				102	*	41.66		-2.103	-9.305		21.02	A
	MOTA	246	0					43.75		-2.103	-8.507		19.38	A
	ATOM	247	N			103							20.87	A
	ATOM	248	CA	ALA				43.83		-3.249	-8.035 -7.671		19.23	A
55	ATOM	249	CB	ALA				45.28		-3.571	-7.671			A
	MOTA	250	C			103		42.91		-3.629	-6.872		19.92	
	ATOM	251	0			103		42.70		-4.815	-6.628		20.38	A
	ATOM	252	N			104		42.36		-2.643	-6.175		18.12	A
	ATOM	253	CA	THR	А	104		41.51	1	-2.927	-5.018	T.00	17.15	A

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	ATOM	254	ĊВ	THR	Α	104		42,212	-2.484	-3.717	1.00 19.54	A
	ATOM	255	OG1	THR	Α	104		42.456	-1.070	-3.773	1.00 19.26	Α
								43.536	-3.219	-3.529	1.00 17.02	A
	ATOM	256		THR							•	
	MOTA	257	С	THR	Α	104		40.159	-2.247	-5.026	1.00 19.44	A
5	ATOM	258	0	THR	Α	104		39.259	-2.648	-4.285	1.00 18.70	Α
_		259	N	SER				40.034	-1.207	-5.847	1.00 19.65	Α
	MOTA											
	MOTA	260	CA	SER	Α	105		38.819	-0.400	-5.967	1.00 19.37	A
	ATOM	261	CB	SER	Α	105		37.598	-1.304	-6.173	1.00 21.81	A
	ATOM	262	OG	SER	Δ	105		36.431	-0.539	-6.412	1.00 23.01	A
10			C	SER				38.644	0.447	-4.701	1.00 18.99	A
10	MOTA	263										
	MOTA	264	0	SER	А	105		37.602	1.070	-4.488	1.00 18.66	Α
	MOTA	265	N	ARG	Α	106		39.674	0.468	-3.861	1.00 16.84	A
	ATOM	266	CA	ARG				39.655	1.267	-2.634	1.00 16.21	Α
								40.827	0.886	-1.723	1.00 16.41	A
	MOTA	267	CB	ARG								
15	ATOM	268	CG	ARG	Α	106		40.619	-0.367	-0.906	1.00 15.49	A
	MOTA	269	CD	ARG	Α	106		41.887	-0.755	-0.170	1.00 17.43	A
	ATOM	270	NE	ARG				41.620	-1.792	0.824	1.00 20.47	A
										1.371	1.00 20.24	A
	MOTA	271	CZ	ARG				42.548	-2.568			
	MOTA	272	NH1	ARG	Α	106		43.821	-2.433	1.017	1.00 17.80	A
20	ATOM	273	NH2	ARG	Α	106		42.198	-3.468	2.285	1.00 20.14	A
	ATOM	274	С	ARG				39.785	2.746	-2.981	1.00 17.37	Α
											1.00 17.75	A
	MOTA	275	0	ARG				40.514	3.103	-3.902		
	ATOM	276	N	GLU	Α	107		39.085	3.599	-2.240	1.00 16.06	A
	ATOM	277	CA	GLU	Α	107		39.156	5.039	-2.461	1.00 20.80	A
25	ATOM	278	СВ	GLU				37.779	5.694	-2.337	1.00 22.93	Α
23								36.711	5.171	-3.269	1.00 30.87	Α
	MOTA	279	CG	GLU								
	ATOM	280	CD	GLU	Α	107		35.431		-3.148	1.00 32.40	A
	ATOM	281	OE1	GLU	Α	107		35.262	6.939	-3.923	1.00 33.74	Α
	ATOM	282	OF2	GLU	Δ	107		34.608	5.654	-2.263	1.00 36.00	Α
20									5.678	-1.410	1.00 18.93	A
30	ATOM	283	С	GLU				40.053				
	ATOM	284	0	GLU	Α	107		39.891	5.427	-0.220	1.00 19.21	A
	ATOM	285	N	TYR	Α	108		40.988	6.507	-1.852	1.00 16.70	Α
	ATOM	286	CA	TYR				41.883	7.209	-0.942	1.00 15.86	Α
								43.325	6.728	-1.104	1.00 15.30	A
	MOTA	287	CB	TYR								
35	ATOM	288	CG	TYR	Α	108		43.593	5.328	-0.612	1.00 16.33	A
	ATOM	289	CD1	TYR	Α	108		43.765	5.066	0.746	1.00 16.36	A
	ATOM	290	CE1					44.046	3.769	1.201	1.00 18.48	Α
								43.701	4.268	-1.511	1.00 13.25	А
	ATOM	291	CD2	TYR								
	ATOM	292	CE2	TYR	Α	108		43.980	2.981	-1.075	1.00 17.28	A
40	ATOM	293	CZ	TYR	Α	108		44.152	2.736	0.276	1.00 19.17	Α
	ATOM	294	ОН	TYR	Δ	108		44.440	1.461	0.688	1.00 19.38	Α
				TYR				41.850	8.687	-1.292	1.00 16.80	A
	ATOM	295	C									A
	MOTA	296	0	TYR				41.560	9.058	-2.431	1.00 15.22	
	MOTA	297	N	ALA	Α	109		42.132	9.528	-0.306	1.00 14.61	A
45	ATOM	298	CA	ALA	Α	109		42.207	10.957	-0.539	1.00 14.30	Α
73				ALA				41.671	11.726	0.661	1.00 14.78	Α
	MOTA	299	СВ									A
	ATOM	300	С	ALA				43.713	11.136	-0.667	1.00 16.79	
	ATOM	301	0	ALA	Α	109		44.450	10.983	0.317	1.00 16.52	Α
	ATOM	302	N	ILE				44.182	11.410	-1.881	1.00 14.80	Α
50								45.609		, -2.093	1.00 15.80	A
50	ATOM	303	CA	ILE								•
	MOTA	304	CB	ILE	Α	110		46.065	10.863	-3.396	1.00 16.85	A
	ATOM	305	CG2	ILE	Α	110		47.550	11.098	-3.632	1.00 16.80	A
	ATOM	306		ILE				45.774	9.358	-3.284	1.00 17.76	A
									8.513	-4.437	1.00 16.07	A
_	ATOM	307		ILE				46.308				A
55	MOTA	308	С			110		46.004	13.045	-2.129	1.00 17.78	
	ATOM	309	0	ILE	Α	110		45.534	13.813	-2.976	1.00 16.24	A
	ATOM	310	N	LYS	Α	111		46.846	13.435	-1.177	1.00 16.15	A
				LYS			-	47.326	14.808	-1.100	1.00 17.20	А
	ATOM	311	CA									A
	ATOM	312	CB	ГXS	A	111		47.700	15.176	0.344	1.00 17.41	А

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	MOTA	313	CG	LYS	Α	111		48.350	16.547	0.464	1.00	20.71		Α
	ATOM	314	CD	LYS	Α	111	•	48.585	16.971	1.910		24.25		Α
	ATOM	315	CE	LYS				47.288	17.381	2.598		29.46		A
	ATOM	316	NZ			111		47.516	17.866	4.000		30.50		A
5	ATOM	317	С	LYS				48.551	14.890	-1.994		16.41		Α
,	ATOM	318	Õ	LYS				49.509	14.137	-1.813		18.20		
		319												A
	ATOM		N	ΙŢΕ				48.509	15.798	-2.963		15.87		A
	ATOM	320	CA	ILE				49.606	15.967	-3.907		17.28		A
	MOTA	321	CB	ILE				49.079	15.911	-5.358		16.43		A
10	MOTA	322		ILE				50.235	15.998	-6.341		15.12		A
	ATOM	323	CG1	ILE				48.293	14.609	-5.565		16.82		A
	ATOM	324		ILE				47.580	14.511	-6.904		18.47		A
	ATOM	325	С	ILE				50.307	17.301	-3.663		19.03		A
	ATOM	326	0	ILE	A	112		49.669	18.350	-3.635		19.15		A
15	ATOM	327	N	LEU .	Α	113		51.622	17.245	-3.472	1.00	20.22		A
	ATOM	328	CA	LEU	А	113		52.416	18.442	-3.214	1.00	22.36		A
	ATOM	329	CB	LEU .	Α	113		52.995	18.397	-1.794	1.00	22.13		A
	ATOM	330	CG	LEU .	Α	113		52.042	18.063	-0.646	1.00	22.46		Α
	ATOM	331	CD1	LEU .	Α	113		51.866	16.557	-0.553	1.00	23.81		Α
20	ATOM	332	CD2	LEU .	Α	113		52.603	18.595	0.660	1.00	23.68		Α
	ATOM	333	С	LEU	Α	113		53.560	18.547	-4.215	1.00	23.37		Α
	ATOM	334	0	LEU				54.300	17.586	-4.424	1.00	23.11		Α
	ATOM	335	N	GLU .				53.706	19.714	-4.834	1.00	23.88		A
	ATOM	336	CA	GLU				54.771	19.920	-5.806		26.00		Ά
25	ATOM	337	СВ	GLU				54.435	21.111	-6.706		27.74		A
23	ATOM	338	CG	GLU				55.533	21.452	-7.696		35.07		A
	ATOM	339	CD	GLU				55.220	22.696	-8.497		39.24		A
	ATOM	340		GLU				54.808	23.703	-7.885		41.45		A
	ATOM	341		GLU .				55.395	22.670	-9.736		44.05		A
30	ATOM	342	C	GLU .				56.087	20.163	-5.067		24.37		A
30		343	0	GLU .				56.186	21.071	-4.238		24.43		A
	MOTA							57.096	19.350	-5.360		24.10		A
	ATOM	344	N	LYS .				58.376	19.493	-4.678		24.93		A
	ATOM	345	CA	LYS .					18.373	-5.103		23.72		A
25	ATOM	346	CB	LYS .		-		59.339		-4.308		23.09		A
35	ATOM	347	CG	LYS				59.139	17.080			21.92		A
	ATOM	348	CD	LYS .				60.064	15.944	-4.743				A A
	ATOM	349	CE	LYS .				59.691	15.400	-6.117		22.42		
	ATOM	350	NZ	LYS				60.447	14.150	-6.448		19.71		A
	ATOM	351	С	LYS .				59.031	20.858	-4.868		26.87		A
40	ATOM	352	0	LYS				59.492	21.469	-3.903		26.17		A.
	MOTA	353	N	ARG				59.058	21.348	-6.102		28.73		A
	ATOM	354	CA	ARG :				59.678	22.638	-6.380		29.66		A
	ATOM	355	CB	ARG			•	59.533	22.980	-7.868		31.29		A
	ATOM	356	CG	ARG .				60.047	24.361	-8.267		33.19		A
45	ATOM	357	CD	ARG .				61.368	24.710	-7.590		35.13		A
	ATOM	358	NE	ARG .				62.329	23.612	-7.618		36.42		A
	ATOM	359	CZ	ARG .				63.510	23.648	-7.009		36.18		A
	ATOM	360	NH1	ARG .	Α	116		63.871	24.729	-6.332		36.12		A
	ATOM	361	NH2	ARG .	Α	116		64.324	22.602	-7.067		35.77	,	A
50	ATOM	362	С	ARG .	A	116		59.097	23.761	-5.519		29.70	1	A
	MOTA	363	0	ARG .	Α	116		59.843	24.515	-4.889	1.00	29.16	1	Α
	MOTA	364	N	HIS .				57.773	23.862	-5.472	1.00	27.22		Α
	ATOM	365	CA	HIS :				57.126	24.903	, -4.681	1.00	26.33		A
	ATOM	366	СВ	HIS.				55.606	24.835	-4.848	1.00	28.41	1	A
55	ATOM	367	CG	HIS.				54.881	26.005	-4.258	1.00	31.82		Α
	ATOM	368		HIS.				55.309	27.249	-3.935		33.19	3	A
	ATOM	369		HIS .				53.536	25.974	-3.961		34.30		A
	ATOM	370		HIS				53.165	27.148	-3.480		34.58		A
	ATOM	371		HIS				54.222	27.940	-3.455		35.18		A
					•									

	ATOM	372	С	HIS I	A 117		57.47,7	24.780	-3.202	1.00	26.22	A
	ATOM	373	0	HIS A	A 117	•	57.737	25.776	-2.534		25.67	•
	ATOM	374	N	ILE A	A 118		57.469	23.554	-2.689	1.00		A.
	ATOM	375	CA	ILE A	A 118		57.792	23.315	-1.285	1.00		A
5	ATOM	376	СВ	ILE A			57.711	21.812	-0.952	1.00		A
	ATOM	377	CG2				58.374	21.533	0.389	1.00		A
	ATOM	378	CG1				56.246	21.362	-0.959	1.00		A
	ATOM	379		ILE A			56.066	19.858	-0.834	1.00		· A
	ATOM	380	C		A 118		59.195	23.821	-0.958	1.00		A
10	ATOM	381	ō	ILE A			59.402	24.495	0.048	1.00		A
	ATOM	382	N	ILE A			60.153	23.489	-1.815	1.00		A
	ATOM	383	CA	ILE A			61.534	23.913	-1.619	1.00		A
	ATOM	384	CB	ILE A			62.467	23.250	-2.664	1.00		A
	ATOM	385		ILE A			63.858	23.890	-2.617	1.00		A
15	ATOM	386	CG1				62.540	21.738	-2.395	1.00		A
	ATOM	387		ILE A			63.327	20.945	-3.439	1.00		A
	ATOM	388	C	ILE 2			61.667	25.435	-1.705	1.00		A
	ATOM	389	Ö	ILE A			62.330	26.051	-0.872		24.78	A
	ATOM	390	N	LYS A			61.028	26.039	-2.704	1.00		A
20	ATOM	391	CA	LYS A			61.100	27.489	-2.879	1.00		A
	ATOM	392	СВ	LYS A			60.242	27.940	-4.060	1.00		A
	ATOM	393	CG	LYS A			60.674	27.407	-5.409	1.00		A
	ATOM	394	CD	LYS A			59.765	27.950	-6.512	1.00		A
	ATOM	395	CE	LYS A			58.294	27.636	-6.218	1.00		A
25	ATOM	396	NZ	LYS A			57.363	28.155	-7.252	1.00		A
	ATOM	397	С	LYS A			60.647	28.247	-1.638	1.00		A
	ATOM	398	0	LYS A			61.303	29.198	-1.217	1.00		A
	ATOM	399	N	GLU A	121		59.527	27.825	-1.055	1.00		A
	ATOM	. 400	CA	GLU A	121		58.986	28.488	0.128	1.00	30.33	A
30	ATOM	401	CB	GLU A	121		57.455	28.416	0.117	1.00	33.04	A
	ATOM	402	CG	GLU A	121		56.794	29.021	-1.120	1.00	36.45	A
	ATOM	403	CD	GLU A	121		57.221	30.456	-1.373	1.00	39.88	A
	ATOM	404	OE1	GLU A	121		57.200	31.264	-0.420	1.00	40.53	A
	ATOM	405	OE2	GLU A	121		57.573	30.778	-2.529	1.00	13.24	A
35	ATOM	406	С	GLU A	121		59.511	27.930	1.451	1.00	30.37	A
	ATOM	407	0	GLU F	121		58.946	28.204	2.513	1.00	31.24	Α
	ATOM	408	N	ASN A			60.588	27.151	1.390	1.00 2		A
	ATOM	409	CA	ASN A			61.183	26.573	2.594	1.00 2		A
	ATOM	410	CB	ASN A			61.836	27.673	3.436	1.00	-	A
40	ATOM	411	CG	ASN A			62.945	28.395	2.698	1.00		A
	ATOM	412		ASN A			62.697	29.143	1.754	1.00		A
	ATOM	413		ASN F			64.181	28.169	3.127	1.00		A
	MOTA	414	С	ASN A			60.157	25.835	3.456	1.00 2		A
4.5	ATOM	415	0	ASN A			60.085	26.055	4.663	1.00 2		A
45	ATOM	416		LYS F			59.375	24.955	2.842	1.00 2		A
	ATOM	417	CA	LYS A			58.358	24.210	3.574	1.00 2		A
	ATOM	418	CB	LYS A			57.031	24.248	2.810	1.00 2		A
	ATOM	419	CG	LYS A			56.475	25.645	2.599	1.00 2		A
50	ATOM	420	CD	LYS A			56.253	26.354	3.927	1.00 2		A
50	MOTA	421	CE	LYS A			55.822	27.796	3.716	1.00 3		A
	MOTA	422	NZ	LYS A			55.756	28.540	5.004	1.00 3		A
	ATOM	423	C	LYS A			58.748	22.759	3.821	1.00 2		A
	ATOM	424	0	LYS A			57.924	21.960	4.264	1.00 2		A
55	ATOM	425	N	VAL A			59.997	22.412	3.535	1.00 2		A
رر	ATOM	426	CA	VAL A			60.439	21.039	3.730	1.00 2		A n
	ATOM ATOM	427 428	CB CG1	VAL A			61.922	20.850 19.407	3.328 3.573	1.00 1		A A
	ATOM	428 429		VAL A			62.346 62.104	21.195	1.853	1.00 1		A A
	ATOM	430	CGZ	VAL A			60.236		5.163	1.00 1		A
	AION	400	J	AVD W	124		00.236	20.561	2.103	1.00 1		A

	3 =014	421	_								
	ATOM	431	0		124		59.841	19.418		1.00 20.02	A
	ATOM	432	N	PRO F	125		60.513	21.422	6.159	1.00 20.01	A
	ATOM	433	CD	PRO P	125		61.178	22.738	6.118	1.00 18.69	A
	ATOM	434	CA	PRO F	125		60.318	20.979	7.544	1.00 19.88	A
5	ATOM	435	СВ	PRO F			60.793	22.180	8.363	1.00 19.95	A
,	ATOM	436	CG	PRO F		•	61.839	22.805	7,479		
										1.00 18.85	A
	ATOM	437	С	PRO F			58.848	20.642	7.824	1.00 19.76	A
	ATOM	438	0	PRO P			58.544	19.700	8.550	1.00 16.99	A
	ATOM	439	N	TYR P			57.947	21.418	7.235	1.00 18.98	Α
10	MOTA	440	CA	TYR F	126		56.516	21.220	7.435	1.00 21.97	Α
	ATOM	441	CB	TYR A	126		55.752	22.448	6.933	1.00 25.17	A
	MOTA	442	CG	TYR A	126		56.040	23.690	7.748	1.00 30.98	A
	MOTA	443	CD1	TYR A			55.438	23.886	8.991	1.00 33.95	A
	ATOM	444		TYR A			55.721	25.015	9.763	1.00 36.60	A
15	ATOM	445		TYR A			56.938	24.657	7.292	1.00 35.43	A
13											
	ATOM	446		TYR A			57.231	25.792	8.058		A
	MOTA	447	CZ	TYR A			56.618	25.962	9.291	1.00 37.40	A
	MOTA	448	ОН	TYR A	126		56.903	27.073	10.052	1.00 40.85	A
	MOTA	449	С	TYR A	126	-	55.990	19.956	6.762	1.00 21.35	A
20	MOTA	450	0	TYR A	126		55.265	19.175	7.383	1.00 20.49	A
	MOTA	451	N	VAL A	127		56.354	19.746	5.501	1.00 18.16	A
	ATOM	452	CA	VAL A	127		55.892	18.562	4.790	1.00 17.58	A
	ATOM	453	CB	VAL A			56.308	18.596	3.308	1.00 17.45	A
	ATOM	454		VAL A			55.786	17.350	2.600	1.00 17.97	A
25				VAL A		-	55.751			1.00 17.97	
25	ATOM	455						19.850	2.641		A
	ATOM	456	C	VAL A			56.459	17.306	5.448	1.00 18.39	A
	ATOM	457.		VAL A			55.769	16.298	5.583	1.00 18.14	A
	ATOM	458	N	THR A	-		57.716	17.381	5.869	1.00 17.50	A
	MOTA	459	CA	THR A	128		58.375	16.260	6.530	1.00 18.54	А
30	MOTA	460	CB	THR A	128		59.861	16.586	6.805	1.00 18.01	A
	ATOM	461	OG1	THR A	128		60.537	16.804	5.559	1.00 21.14	A
	ATOM	462	CG2	THR A	128		60.536	15.446	7.545	1.00 17.95	A
	ATOM	463	C	THR A			57.676	15.941	7.856	1.00 19.49	A
	ATOM	464	Ö	THR A			57.438	14.776	8.179	1.00 18.76	A
35	ATOM	465		ARG A			57.345	16.981	8.619	1.00 19.60	A
33			N						9.904	1.00 19.00	A
	MOTA	466	CA	ARG A			56.673	16.804			
	ATOM	467	СВ	ARG A			56.534	18.144	10.621	1.00 21.33	A
	ATOM	468	CG	ARG A			55.948	18.029	12.023	1.00 28.02	A
	ATOM	469	CD	ARG A			55.721	19.404	12.597	1.00 31.25	A
40	ATOM	470	NE	ARG A	129		56.940	20.205	12.560	1.00 37.78	A
	ATOM	471	CZ	ARG A	129		56.962	21.524	12.391	1.00 40.10	A
	ATOM	472	NH1	ARG A	129		55.828	22.197	12.239	1.00 40.03	· A
	ATOM	473		ARG A			58.119	22.170	12.374	1.00 44.58	А
	ATOM	474	С	ARG A			55.288	16.186	9.729	1.00 20.08	A
45	ATOM			ARG A			54.891		10.496		A
		476		GLU A		•	54.553	16.654	8.724	1.00 18.79	A
	ATOM		N								
	ATOM	477	CA	GLU A			53.222	16.125	8.454	1.00 20.10	A
	ATOM	478	CB	GLU A			52.638	16.749	7:183	1.00 19.92	A
	ATOM	479	CG	GLU A			51.350	16.087	6.708	1.00 27.85	A
50	MOTA	480	CD	GLU A	130		50.581	16.933	5.707	1.00 29.72	A
	ATOM	481	OE1	GLU A	130		51.216	17.528	4.814	1.00 33.46	, A
	ATOM	482	OE2	GLU A	130		49.339	16.996	5.807	1.00 30.74	, A
	ATOM	483	С	GLU A			53.301	14.615	8.295	1.00 19.81	Α
	ATOM	484	ō	GLU A			52.553	13.875	8.935	1.00 18.37	A
55	ATOM	485	N	ARG A			54.219	14.162	7.447	1.00 20.41	A
	ATOM	486	CA	ARG A			54.397	12.735	7.202	1.00 22.45	A
							55.442			1.00 25.16	A
	ATOM	487	CB	ARG A							
	ATOM	488	CG	ARG A			55.742	11.043	5.840	1.00 28.75	A
	ATOM	489	CD	ARG A	131		56.736	10.837	4.708	1.00 33.75	· A

														•
	ATOM	490	NE	ARG	Α	131		57.020	9.41	15	4.520		40.07	Α
	ATOM	491	CZ	ARG	Α	131		57.756	8.93	15	3.532		43.07	A
	ATOM	492	NH1	ARG	A	131		58.293	9.72	21	2.625		44.91	A
	ATOM	493	NH2	ARG	A	131		57.955	7.60	06	3.449	1.00	44.45	A
5	ATOM	494	·C	ARG	Α	131		54.820	11.98	82	8.466		23.24	A
	ATOM	495	0	ARG	Α	131		54.241	10.94	48	8.804		23.86	A
`	ATOM	496	N ·	ASP				55.831	12.49		9.160		21.99	A
	ATOM	497	CA	ASP	Α	132		56.318	11.85		10.370		22.04	A
	ATOM	498	СВ	ASP	Α	132		57.570	12.5	64	10.888		23.72	A
10	ATOM	499	CG	ASP	Α	132		58.750	12.44	42	9.932		27.77	A
	ATOM	500		ASP				58.681	11.62		8.989		27.34	A
	MOTA	501	OD2	ASP	Α	132		59.753	13.10		10.128		28.70	A
	MOTA	502	С	ASP	A	132		55.258	11.7		11.474		21.69	A
	MOTA	503	0	ASP				55.077	10.72		12.092		22.75	A
15	ATOM	504	N	VAL	A	133		54.551	12.8		11.725		19.54	A
	MOTA	505	CA	VAL	A	133		53.525	12.8		12.759		18.52	A
	ATOM	506	CB	VAL	A	133		52.908	14.2		12.990		19.26	Ą
	MOTA	507	CG1	VAL	A	133		51.708	14.13		13.918		18.79	A
	MOTA	508	CG2	VAL				53.953	15.1		13.604		18.80	A
20	ATOM	509	С	VAL				52.419	11.8		12.398		19.46	A
	MOTA	510	0	VAL	A	133		52.073	10.9		13.200		19.94	Α,
	MOTA	511	N			134		51.878	11.9		11.187		19.15	A
	ATOM	512	CA	MET				50.807	11.0		10.792		21.25	A
	ATOM	513	CB	MET				50.309	11.3		9.383		17.34	. A
25	ATOM	514	CG			134		49.615	12.7		9.302		20.00	· A A
	MOTA	515	SD			134		48.643	12.9		7.798		24.21	. A
	MOTA	516	CE			134		47.033	12.4		8.400	1.00	23.20 22.43	A
	ATOM	517	C.			134		51.203	9.5		10.881		23.82	A
	MOTA	518	0			134		50.384	8.7		11.249		23.02	A
30	MOTA	519	N			135		52.454	9.2		10.556		26.13	A
	MOTA	520	CA			135		52.939	7.8		10.615		26.17	A
	MOTA	521	CB			135		54.356	7.7 8.1		8.673		31.91	Α.
	MOTA	522	OG			135		54.383	7.3		12.045		26.58	A
	MOTA	523	Ç			135		52.957 52.926	6.1		12.261		26.42	A
35	ATOM	524	0			135		53.014	8.2		13.018		25.65	A
	MOTA	525	N			136 136	,	53.056	7.8		14.425		27.47	A
	ATOM	. 526	CA	ARG				53.823	8.9		15.238		27.97	А
	ATOM	527	CB			136		55.283	9.0		14.857		32.00	А
40	ATOM	528	CG			136		55.904	10.2		15.664		33.03	Α.
40	ATOM	529 530	CD NE			136		55.602	10.0		17.084		36.11	A
•	MOTA	530	CZ			136		55.867	10.9		18.007	1.00	39.74	A
	ATOM ATOM	532		ARG				56.449	12.1		17.661	1.00	40.55	· A
	ATOM	533		ARG				55.540	10.7		19.276	1.00	.36.72	A
45	ATOM	534	C			136		51.667	7.7		15.036	1.00	26.38	A
43	ATOM	535	0			136		51.516	7.1		16.106		27.06	A
	ATOM	536	N	T.E.U	A	137		50.655	8.2		14.360	1.00	24.77	· A
	ATOM	537	CA			137		49.294	8.1		14.870	1.00	24.70	A
	ATOM	538	CB			137		48.483	9.3	363	14.371	1.00	24.52	A
50	ATOM	539	CG			137		49.050	10.7	60	14.662		26.67	A
50	MOTA	540		LEU				48.075	11.8	313	14.141	1.00	27.25	A
	ATOM	541		LEU				49.279	10.9	945	16.155		27.09	A
	ATOM	542	C			137		48.592	6.8	368	14.473		25.20	A
	ATOM	543	ō			137		48.619	6.4	169	13.309		25.99	A
55	ATOM	544	N			138		47.971	6.2		15.451		21.89	A
	ATOM	545	CA			138		47.239	4.9	977	15.219		21.35	A
	ATOM	546	CB			138		48.124	3.7		15.523		22.14	A
	ATOM	547	CG	ASP	Α	. 138		47.432			15.201		24.90	A
	ATOM	548	OD1	L ASP	Α	138		46.631	2.4	123	14.241	1.00	24.78	A

	ATOM	549	OD2	ASP	A	138		47.691	1.443	15.897	1.00 25.39	A
	ATOM	550	С	ASP	Α	138		46.031	4.991	16.138	1.00 20.47	Α
	ATOM	551	0	ASP	Α	138	•	45.967	4.248	17.118	1.00 19.06	A
	ATOM	552	N	HIS	Α	139		45.075	5.852	15.810	1.00 18.27	A
5	ATOM	553	CA	HIS				43.869	6.016	16.606	1.00 18.21	A
	ATOM	554	СВ			139		44.096	7.157	17.612	1.00 15.84	A
•	ATOM	555	CG	HIS				42.985	7.332	18.600	1.00 15.24	A
	ATOM	556		HIS				42.884	6.964	19.900	1.00 13.24	A
	ATOM	557		HIS				41.791	7.943	18.280	1.00 13.37	A
10	ATOM	558		HIS				41.002	7.944	19.341	1.00 14.74	A
10	ATOM	559		HIS				41.641	7.356	20.336	1.00 14.15	A
	ATOM	560	C	HIS				42.715	6.330	15.654	1.00 14.15	A
		561		HIS				42.713	7.080	14.693		A
	ATOM		0						5.767		1.00 20.80 1.00 18.32	
15	ATOM	562	И	PRO				41.527		15.913	•	A
15	ATOM	563	CD	PRO				41.143	4.984	17.100	1.00 16.71	A
	ATOM	564				140		40.367	6.001	15.048	1.00 17.43	A
	MOTA	565	CB			140.		39.273	5.157	15.704	1.00 16.64	A
	MOTA	566	CG	PRO				39.643	5.204	17.152	1.00 18.43	A
'	MOTA	567	С	PRO	•			39.914	7.441	14.803	1.00 18.77	A
20	ATOM	568	0	PRO				39.207	7.695	13.831	1.00 19.88	A
	MOTA	569	N	PHE				40.301	8.381	15.664	1.00 17.14	A
	ATOM	570	CA	PHE				39.874	9.767	15.477	1.00 16.42	A
	MOTA	571	CB	PHE	Α	141		39.568	10.422	16.836	1.00 14.60	A
	MOTA	572	CG	PHE				38.386	9.817	17.556	1.00 15.26	A
25	MOTA	573		PHE				37.335	9.234	16.842	1.00 14.78	A
	MOTA	574	CD2	PHE	Α	141		38.297	9.880	18.942	1.00 13.70	A
	MOTA	575	CE1	PHE	Α	141		36.215	8.727	17.502	1.00 16.94	A
	MOTA	576	CE2	PHE	Α	141		37.178	9.375	19.615	1.00 15.75	A
	ATOM	577	CZ	PHE	Α	141		36.135	8.799	18.893	1.00 16.89	A
30	ATOM	578	С	PHE	Α	141		40.857	10.641	14.694	1.00 16.15	A
	ATOM	579	Ο.	PHE	Α	141		40.799	11.871	14.761	1.00 17.35	A
	ATOM	580	N	PHE	Α	142		41.748	10.011	13.941	1.00 15.88	A
	ATOM	581	CA	PHE	Α	142		42.727	10.756	13.154	1.00 17.89	Α
	ATOM	582	CB	PHE	Α	142		44.115	10.645	13.793	1.00 17.57	A
35	ATOM	583	CG	PHE	Α	142		44.240	11.371	15.103	1.00 18.74	A
	ATOM'	584	CD1	PHE	Α	142		44.559	12.726	15.135	1.00 17.77	A
	ATOM	√585	CD2	PHE	Α	142		43.997	1.0.711	16.304	1.00 18.74	A
	ATOM	586	CE1	PHE	Α	142		44.632	13.417	16.347	1.00 15.77	A
	ATOM	587		PHE				44.065	11.393	17.522	1.00 17.56	A
40	ATOM	588	CZ	PHE	-			44.383	12.747	17.542	1.00 17.14	Α
	ATOM	589	С	PHE				42.793	10.231	11.729	1.00 19.12	A
	ATOM	590	0	PHE				42.659	9.030	11.504	1.00 20.01	A
	ATOM	591	N	VAL	Α	143		42.978	11.135	10.769	1.00 18.72	A
	ATOM	592	CA	VAL	Α	143		43.102	10.735	9.371	1.00 18.52	A
45	ATOM	593	CB	VAL	_			43.294	11.961	8.440	1.00 20.66	A
	ATOM	594		VAL				43.843	11.521	7.080	1.00 21.29	Α
	ATOM	595		VAL				41.958	12.673	8.252	1.00 22.97	A
	ATOM	596	C	VAL				44.342	9.865	9.330	1.00 18.68	A
	ATOM	597	ō	VAL				45.355	10.199	9.943	1.00 18.42	· A
50	ATOM	598	N	LYS				44.259	8.745	8.623	1.00 18.30	A
50	ATOM	599	CA	LYS				45.384	7.824	8.535	1.00 18.78	Α
	ATOM	600 .		LYS				44.889	6.373	8.608	1.00 22.27	Α
	ATOM	601	CG	LYS				46.017	5.340	8.557	1.00 29.72	. A
	ATOM	602	CD	LYS				45.491	3.912	8.674	1.00 23.72	A
55	ATOM	603	CE	LYS				46.631	2.896	8.577	1.00 34.10	A
در		604	NZ	LYS				46.138	1.484	8.629	1.00 37.07	A
	ATOM		NZ C	LYS				46.192		7.261	1.00 39.02	A
	ATOM	605						45.643	8.002		1.00 18.18	A
	ATOM	606	O N	LYS					8:314	6.200	1.00 16.18	A
	MOTA	607	N	LEU	A	TAO		47.502	7.816	7.385	1.00 10.79	A

	ATOM	608	CA	LEU ·	A 145	48.411	7.900	6.251	1.00 17.45	A
	ATOM	609		LEU Z			8.653	6.641	1.00 18.82	A
	ATOM	610	CG	LEU			8.902	5.549	1.00 20.23	A
	ATOM	611		LEU :			9.799	6.093	1.00 18.83	A
5	ATOM	612		LEU			7.581	5.069	1.00 19.79	A
3		613		LEU I			6.450	5.907	1.00 19.19	A
	ATOM		C				5.772	6.659	1.00 17.36	A
	ATOM	614	0	LEU .						A
	MOTA	615	N		A 146		5.972	4.782	1.00 17.28	
	ATOM	616	CA		A 146		4.593	4.358	1.00 17.57	A
10	MOTA	617	СВ		A 146		4.098	3.486	1.00 17.74	. A
	MOTA	618	CG		A 146		3.926	4.214	1.00 17.50	A
٠.	ATOM	619		TYR I			4.995	4.377	1.00 16.50	A
	ATOM	620	CE1				4.827	5.039	1.00 17.10	Α
	MOTA	621	CD2	TYR I	A 146	45.620	2.686	4.735	1.00 18.28	A
15	ATOM	622	CE2	TYR .	A 146	44.411	2.506	5.399	1.00 19.84	A
	MOTA	623	CZ	TYR :	A 146	43.547	3.576	5.544	1.00 17.53	A
	ATOM	. 624	ОН	TYR .	A 146	42.342	3.376	6.169	1.00 20.67	A
	ATOM	625	С	TYR .	A 146	49.735	4.376	3.582	1.00 18.72	A
	ATOM	626	0	TYR .	A 146	50.382	3.338	3.715	1.00 19.51	A
20	MOTA	627	N	PHE.	A 147	50.110	5.350	2.765	1.00 18.09	Α
_,	ATOM	628	CA		A 147		5.203	1.952	1.00 17.20	A
	ATOM	629	СВ		A 147		4.258	0.783	1.00 16.77	Α
	ATOM	630	CG		A 147		4.699	-0.070	1.00 17.75	A
	ATOM	631		PHE .			5.752	-0.975	1.00 16.58	A
25	ATOM	632		PHE .			4.075	0.053	1.00 18.07	A
23	ATOM	633		PHE .			6.178	-1.742	1.00 19.62	A
		634		PHE .			4.492	-0.710	1.00 18.56	A
	MOTA	635	CE2		A 147		5.546	-1.610	1.00 19.27	A
	ATOM							1.395	1.00 17.13	A
20	MOTA	636	C		A 147		7.528	1.452	1.00 14.43	A
30	MOTA	637	0		A 147			0.854	1.00 17.12	A
	ATOM	638	N		A 148		6.534	0.834	1.00 17.12	A
	ATOM	639	CA		A 148		7.718	1.197	1.00 17.50	A
	MOTA	640	CB.		A 148		8.531			A
	MOTA	641	OG1				7.760	1.537	1.00 18.83	A
35	MOTA	642	CG2		A 148		8.897	2.472	1.00 19.60	
	MOTA	643	С		A 148		7.262	-0.946	1.00 20.31	A
	ATOM	644	0		A 148		6.124	-0.991	1.00 18.94	A
	MOTA	645	N		A 149		8.149	-1.916	1.00 19.16	A
	MOTA	646	CA		A 149		7.877	-3.073	1.00 18.01	A
40	MOTA	647	CB		A 149		6.801	-3.989	1.00 17.23	A
	MOTA	648	CG	PHE	A 149		7.144	-4.544	1.00 16.88	Α
	ATOM	649		PHE			7.888	-5.712	1.00 18.58	A
	ATOM	650	CD2	PHE	A 149	52.235	6.668	-3.927	1.00 17.31	A
	ATOM	651	CE1	PHE	A 149		8.149	-6.267	1.00 19.26	A
45	MOTA	652	CE2	PHE	A 149	50.972	6.923	-4.470	1.00 19.17	A
	MOTA	653	CZ		A 149		7.663	-5.642	1.00 19.60	Α
	ATOM	654	С		A 149		9.205	-3.774	1.00 20.85	Α
	ATOM	655	0		A 149		10.200	-3.376	1.00 19.76	A
	ATOM	656	N		A 150	4	9.241	-4.782	1.00 19.79	A
50	ATOM	657	CA		A 150		10.481	-5.497	1.00 24.03	A
30	ATOM	658	CB		A 150		11.347	-4.739	1.00 24.45	Α
	ATOM	659	CG		A 150		10.645	-4.414	1.00 26.28	A
	ATOM	660	CD		A 150		11.558	-3.692	1.00 29.02	A
		661		GLN			12.353	-4.321	1.00 27.05	A
55	ATOM	662		GLN			11.449	-2.365	1.00 26.47	A
55	ATOM				A 150		10.203	-6.885	1.00 23.88	A
	ATOM	663	C				9.118	-7.158	1.00 24.79	A
	ATOM	664	0		A 150		11.171	-7.774	1.00 25.88	A
	ATOM	665	N		A 151				1.00 25.00	A
	MOTA	666	CA	ASP	A 151	57.527	11.047	-9.117	1.00 20.49	A

	T. MO14	667				407	33 306				
•	MOTA	667	CB	ASP A				-10.199		24.54	A
	MOTA	668	CG	ASP A	151	55.544	12.336	~10.064	1.00	24.95	A
	ATOM	669	OD1	ASP A	151	56.005	13.379	-9.561	1.00	22.44	A
	ATOM	670	OD2	ASP A	1.51	54.369	12,242	-10.490		25.72	A
5	ATOM	671	С	ASP A		58.515	12.203			28.63	A
,	ATOM	672	ŏ	ASP A		58.890	12.780	-8.194			
										27.83	A
	ATOM	.673	N	ASP A		58.934		-10.426		29.21	A
	ATOM	674	CA	ASP A		59.907		-10.562		31.88	A
	ATOM	675	CB	ASP A	152	60.325	13.792	-12.026	1.00	33.94	A
10	ATOM	676	CG	ASP A	152	61.033	12.564	-12.557	1.00	38.88	A
	ATOM	677	OD1	ASP A	152	61.817	11.959	-11.791	1.00	39.67	A
	ATOM	678		ASP A		60.817		-13.738		41.57	A
	ATOM	679	C	ASP A		59.487		-10.013		30.90	A
1.5	ATOM	680	0	ASP A		60.316	15.735	-9.482		31.69	A
15	ATOM	681	N	GLU A		58.207		-10.107		29.44	A
	ATOM	682	CA	GLU A	153	57.767	16.632	-9.646	1.00	28.69	A
	MOTA	683	CB	GLU A	153	56.984	17.327	-10.766	1.00	32.90	Α
	ATOM	684	CG	GLU A	153	57.451	16.987	-12.183	1.00	40.57	Α
	ATOM	685	CD	GLU A	153	56.920	15.643	-12.675	1.00	45.78	A
20	ATOM	686		GLU A		55,682		-12.760		48.91	A
20	ATOM	687		GLU A		57.736		-12.979		48.95	A
							16.683	-8.372		26.43	
	ATOM	688	C	GLU A		56.929					A
	MOTA	689	0	GLU A		56.947	17.688	-7.660		25.08	A
	ATOM	690	N.	LYS A		56.205	15.610	-8.069		22.39	A
25	MOTA	691	CA	LYS A	154	55.318	15.631	-6.912	1.00	21.43	A
	MOTA	692	CB	LYS A	154	53.861	15.628	-7.398	1.00	20.33	A
	ATOM	693	CG	LYS A	154	53.505	16.716	-8.403	1.00	21.92	A
	ATOM	694	CD	LYS A	154	52.211	16.375	-9.146	1.00	19.70	A
	ATOM	695	CE	LYS A		51.775		-10.077		20.04	A
30	ATOM	696	NZ	LYS A		50.631		-10.951		19.97	A
50		697		LYS A		55.458	14.522	-5.881		20.43	A
	ATOM		С								
	ATOM	698	0	LYS A		55.949	13.426	-6.173		21.13	A
	. ATOM	699	N	LEU A		54.985	14.832	-4.676		19.69	A
	ATOM	700	CA	LEU A	155	54,950	13.900	-3.553		19.10	A
35	ATOM	701	CB	LEU A	155	55.362	14.588	-2.252	1.00	19.65	A
	ATOM	702	CG	LEU A	155	56.740	15.234	-2.129	1.00	21.20	A
	ATOM	703	CD1	LEU A	155	56.848	15.918	-0.770	1.00	23.42	A
	ATOM	704		LEU A		57.816	14.174	-2.277		23.08	, A
	ATOM	705	C	LEU A		53.478	13.507	-3.427		18.87	A
40	ATOM	706		LEU A		52.600	14.348	-3.620		18.61	A
40			0				12.249				
	ATOM	707	И	TYR A		53.209		-3.091		15.02	A
	ATOM	708	CA	TYR A		51.834	11.783	-2.934		16.29	A
	ATOM	709	CB	TYR A		51.470	10.769	-4.029		14.20	A
	MOTA	710	CG	TYR A		51.603	11.273	-5.449		17.29	A
45	ATOM	711	CD1	TYR A	156	52.857	11.429	-6.045	1.00	16.46	A
	ATOM	712		TYR A		52.978	11.884	-7.360	1.00	18.68	Α
	ATOM	713		TYR A		50.474	11.588	-6.202	1.00	16.43	Α
	ATOM	714		TYR A		50.583	12.048	-7.512		16.31	A
		715	CZ			51.835	12.192	-8.083		18.17	A
50	ATOM			TYR A						17.47	
50	ATOM	716	ОН	TYR A		51.941	12.651	-9.371			A
	ATOM	717	С	TYR A		51.657	11.108	-1.572		16.32	A
	ATOM	718	0	TYR A		52.412	10.197	-1.235		16.27	A
	ATOM	719	N	PHE F	157	50.678	11.568	-0.792		15.47	A
	ATOM	720	CA	PHE A	157	50.385	10.966	0.508	1.00	16.66	Α
55	ATOM	721	CB	PHE A		50.324	12.014	1.629	1.00	16.91	A
-	ATOM	722	CG	PHE F		51.631	12.708	1.907		18.96	A
	ATOM	723		PHE A		52.821	12.261	1.340		20.31	A
	ATOM	724		PHE F		51.664	13.829	2.732		21.12	A
										22.08	
	ATOM	725	CEI	PHE F	T 7 2 \	54.025	12.926	1.585	1.00	22.00	A

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	ATOM	726	CE2	PHE A	157	52.865	14.500	2.982	1.00	22.18	A
•	ATOM	727	CZ	PHE A		54.045	14.045	2.405	1.00	21.27	A
		728	c	PHE A		49.016	10.308	0.404	_	16.52	A
	ATOM										
٠.	MOTA	729	Ö	PHE A		48.029	10.979	0.110		17.32	A
5	ATOM	730	N	GLY A	158	48.953	9.002	0.644	1.00	15.97	A
	ATOM	731	CA	GLY A	158	47.684	8.299	0.572	1.00	16.13	A
	ATOM	732	С	GLY A	158	47.000	8.383	1.920	1.00	14.94	A
		733		GLY A		47.445	7.756	2.879		16.28	A
	ATOM		0								
	ATOM	734	N	LEU A		45.915	9.145	1.989		13.50	A
10	MOTA	735	CA	LEU A	159	45.191	9.340	3.241		15.20	A
	ATOM	736	CB	LEU A	159	45.031	10.835	3.517	1.00	14.20	A
	ATOM	737	CG	LEU A	159	46.270	11.726	3.385	1.00	19.00	A
	ATOM	738		LEU A		45.847	13.188	3.477		17.12	A
				LEU A		47.275	11.390	4.471		14.71	A
	ATOM	739								15.53	A
15	ATOM	740	С	LEU A		43.809	8.716	3.232			
	ATOM	741	0	LEU A	. 159	43.232	8.472	2.177		16.05	A
	ATOM	742	N	SER A	160	43.268	8.469	4.418	1.00	15.86	A
	ATOM	743	CA	SER A	160	41.932	7.917	4.498	1.00	19.01	A
	ATOM	744	СВ	SER A		41.566	7.582	5.949	1.00	22.90	A
00						41.901	8.629	6.833		24.18	A
20	MOTA	745	OG	SER A							A
	MOTA	746	С	SER A		40.987	8.968	3.924		20.43	
	MOTA	747	0	SER A	. 160	41.213	10.173	4.062		19.96	A
	ATOM	748	N	TYR A	161	39.945	8.508	3.250		19.20	A
	ATOM	749	CA	TYR A	161	38.975	9.406	2.644	1.00	20.37	A
25	ATOM	750	СВ	TYR A		38.471	8.785	1.332	1.00	20.00	A
23				TYR A		37.314	9.502	0.666		20.72	A
	AŢOM	751·	CG				10.895	0.682		18.22	A
	MOTA	752		TYR A		37.222					
	MOTA	753		TYR A		36.180	11.557	0.029		22.24	A
	MOTA	754	CD2	TYR P	. 161	36.333	8.784	-0.020		20.53	A
30	ATOM	755	CE2	TYR A	161	35.287	9.436	-0.678	1.00	24.24	A.
	ATOM	756	CZ	TYR A		35.218	10.822	-0.648	1.00	22.32	A
	ATOM	757	ОН	TYR A		34.194	11.471	-1.298	1.00	23.03	Α
						37.812	9.681	3.598		20.14	A
	MOTA	758	С	TYR F						19.53	A
	ATOM	759	0	TYR F		36.959	8.819	3.810			
35	MOTA	760	N	ALA A	162	37.791	10.880	4.178		19.92	A
	MOTA	761	CA	ALA A	162	36.721	11.271	5.099		21.07	A
	ATOM	762	СВ	ALA '	162	37.187	12.419	6.002	1.00	19.60	A
	MOTA	763	C	ALA A		35.542	11.712	4.238	1.00	22.07	A
		764	ō	ALA F		35.436	12.875	3.860	1.00	20.66	A
40	ATOM					34.653	10.769	3.945		23.27	A
40	ATOM	765	N	LYS F				3.080		27.12	. A
	ATOM	766	CA	LYS A		33.503	11.017				
	MOTA	767	CB	LYS F		32.663	9.741	2.963		29.68	A
	ATOM	768	CG	LYS A	163	33.455	8.524	2.515		37.67	A
	ATOM	769	CD	LYS A	163	32.556	7.310	2.321	1.00	42.24	Α
45 .		770	CE	LYS F		33.373	6.034	2.185	1.00	44.48	A
75 .		771	NZ	LYS A		34.143	5.735	3.430		44.88	Α
	ATOM					32.581	12.186	3.411		25.78	A
	ATOM	772	С	LYS A							
	ATOM	773	0	LYS I		32.103	12.863	2.506		26.53	A
	ATOM	774	N	ASN F	164	32.327	12.441	4.689		24.57	A
50	ATOM	775	CA	ASN F	164	31.420	13.522	5.033	1.00	23.77	A
	ATOM	776	ĊВ	ASN A		30.610	13.129	6.265	1.00	25.02	A
	ATOM	777	CG	ASN A		29.537	12.101	5.932	1.00	27.54	A
						28.772	12.281	4.983		28.79	A
	ATOM	778		ASN A							A
	ATOM	779		ASN A		29.475	11.024	6.704		27.13	
55	ATOM	780	С	ASN A		31.999	14.931	5.169		24.43	A
	ATOM	781	0	ASN A	164	31.306	15.856	5.589		23.98	A
	ATOM	782	N	GLY A		33.262	15.097	4.795		21.56	A
	ATOM	783	CA	GLY I		33.873	16.414	4.836	1.00	24.39	A
		784	C	GLY A		34.191	17.043	6.181		23.62	A
	MOTA	104	C	GUI A	1 100	54.454				· · · - · -	-

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	ATOM	785	0.	GLY A	165	34.380	16.352	7.177	,1.00	23.26	·A
	ATOM	786		GLU A		34.234	18.373	6.186	1.00	23.22	A
	ATOM	787		GLU A		34.563	19.176	7.362	1.00	24.54	A
	ATOM	788		GLU A		35.055	20.558	6.913	1.00	25.04	A
5	ATOM	789		GLU A		36.419	20.569	6.229	1.00	26.48	A
3		790		GLU A		36.699	21.889	5.517	1.00	30.02	A
	MOTA	791		GLU A		36.081	22.906	5.889	1.00	29.33 .	A
	ATOM	792			166	37.544	21.916	4.596		30.48	A
	ATOM			GLU A		33.436	19.372	8.369		24.44	A
	ATOM	793		GLU A		32.279	19.541	8.001		22.76	A
10	ATOM	794	-			33.791	19.370	9.649		22.95	A
	MOTA	795		LEU A		32.813	19.581	10.707		22.26	A
	MOTA	796		LEU A		33.497	19.481	12.073		22.32	A
	ATOM	797		LEU A		32.706	19.923	13.306		22.04	A
	MOTA	798		LEU A				13.463		19.66	A
15	ATOM	799		LEU A		31.454	19.074			21.17	A
	MOTA	800		LEU A		33.597	19.805	14.537		23.49	A
	ATOM	801		LEU A		32.193	20.971	10.529			A
	ATOM	802		LEU A		31.047	21.209	10.907		23.56	A
	MOTA	803	N	LEU A	168	32.960	21.887	9.948		24.25	
20	ATOM	804	CA	LEU F	168	32.473	23.245	.9.722		26.64	
	ATOM	805	CB	LEU F	168	33.560	24.099	9.066		25.62	A
	MOTA	806	CG	LEU F	168	33.198	25.546	8.707		27.34	A
	ATOM	807	CD1	LEU F	168	32.718	26.296	9.946		26.42	A
	MOTA	808	CD2	LEU A	168	34.418	26.238	8.119		26.74	A
25 ·		809	С	LEU A	168	31.234	23.218	8.829		27.13	A
20	ATOM	810	0	LEU A	168	30.297	23.989	9.030		26.01	A
	ATOM	811	N	LYS A	169	31.233	22.320	7.848		26.41	A
	ATOM	812	CA		169	30.106	22.210	6.934		27.70	A
	ATOM	813	СВ		169	30.324	21.064	5.945		30.49	A
30	ATOM	814	CG		169	29.151	20.854	4.993		32.47	A
30	ATOM ATOM	815	CD		A 169	29.407	19.728	3.998		35.98	A
		816	CE		A 169	29.462	18.372	4.683		38.53	A
	ATOM	817	NZ		A 169	29.622	17.263	3.702		41.00	A
	ATOM	818	C		A 169	28.801	21.985	7.682	1.00	28.12	A
25	ATOM	819	0		A 169	27.785	22.608	7.371	1.00	28.08	Α
35	ATOM	820	N		A 170	28.826	21.094	8.668	1.00	26.53	A
	ATOM	821	CA		A 170	27.624	20.791	9.434	1.00	26.95	A
	ATOM				A 170	27.810	19.476	10.193	1.00	25.03	A
	ATOM	822	CB		A 170	27.898	18.300	9.251		26.65	A
	MOTA	823	CG		A 170	26.745	17.661	8.790	1.00	28.27	A
40	MOTA	824			A 170	26.814	16.642	7.839		26.85	A
	ATOM	825			A 170	29.127	17.884	8.742		27.83	A
	ATOM	826				29.209	16.869	7.792		27.19	Α
*	ATOM	827			A 170	28.049	16.254	7.343		30.02	A
	MOTA	828	CZ		A 170	28.130	15.268	6.382		29.23	A
45	ATOM	829	OH		A 170		21.918	10.376		27.59	A
	MOTA	830	C		A 170	27.229	22.122	10.642		29.25	A
	ATOM	831	0		A 170	26.045		10.882		28.16	. A
	ATOM	832	N		A 171	28.208	22.660	11.763		29.03	. A
	ATOM	833	CA		A 171	27.883	23.770	12.337		27.51	A
50	MOTA	834	CB		A 171	29.151	24.435			27.97	A
	MOTA	835			A 171	28.773	25.705	13.084		26.70	A
	ATOM	836			A 171	29.872	23.458	13.272		24.07	A
	ATOM	837	CD1		A 171	31.163	23.996	13.856			A
	ATOM	838	С		A 171	27.094	24.796	10.944		31.41	A
55	ATOM	839	0		A 171	26.088	25.335	11.407		31.69	A
•	ATOM	840	N		A 172	27.546	25.047	9.719		33.21	
	ATOM	841	CA	ARG	A 172	26.874	26.000	8.844		36.54	A
	ATOM	842	CB		A 172	27.734	26.314			37.73	A A
	ATOM	843	CG	ARG	A 172	29.057	27.011	7.912	Τ.00	0 41.65	А

	ATOM	844	CD	ARG	Α	172	29.708	27.492	6.616	1.00	45.29		A
	ATOM		NE	ARG			31.037	28.070	6.812	1.00	48.51		Α.
	ATOM	846	CZ	ARG			31.314	29.059	7.658		51.53		A
								29.593	8.406		53.75		A
_	ATOM	847		ARG			30.355						
5	MOTA	848		ARG			32.553	29.526	7.748		51.21		A
,	ATOM	849	С	ARG			25.528	25.459	8.378		37.67		Α
	ATOM	850	0	ARG	Α	172	24.550	26.200	8.288	1.00	39.09		Α
	ATOM	851	N	LYS	Α	173	25.481	24.163	8.092	1.00	38.44		A
	ATOM	852	CA	LYS	Α	·173	24.259	23.528	7.619	1.00	39.25		Α
10	ATOM	853	CB.	LYS			24.523	22.061	7.272	1.00	41.89		Α
10	ATOM	854	CG	LYS			23.279	21.298	6.830		45.52		A
								19.808	6.653		49.60		A
	ATOM	855	CD			173	23.557						
	ATOM	856	CE	LYS			24.477	19.530	5.469		52.63		A
	ATOM	857	NZ	LYS	Α	173	23.855	19.894	4.160		54.61		Α
15	ATOM	858	C ·	LYS	Α	173	23.089	23.608	8.595	1.00	39.30		Α
	MOTA	859	0	LYS	Α	173	21.981	23.960	8.201	1.00	39.62		Α
	ATOM	860	N	ILE			23.320	23.282	9.863	1.00	37.96		Α
	ATOM	861	CA	ILE			22.229	23.314	10.833		37.36		Α
		862	CB	ILE			22.159	21.998	11.652		37.44		A
	ATOM												A
20	ATOM	863		ILE			22.058	20.802	10.709		38.37		
	ATOM	864		ILE			23.397	21.850	12.532		37.25		A
	MOTA	865	CD1	ILE	A	174	23.355	20.620	13.418		36.85		A
	, ATOM	866	C ·	ILE	Α	174	22.259	24.492	11.801	1.00	36.71		Α
	ATOM	8 67	0	ILE	A	174	21.448	24.556	12.724	1.00	38.05		Ą
25	ATOM	868	N	GLY			23.185	25.423	11.592	1.00	35.48		À
23	ATOM	869	CA	GLY			23.265	26.585	12.462		35.29		A
							24.053	26.360	13.737		35.06		A
	ATOM	870	C	GLY							37.46		A
	MOTA	871	0	GLY			25.066	27.019	13.970				
	ATOM	872	N	SER			23.581	25.441	14.571		33.94		A
30	MOTA	873	CA	SER	Α	176	24.253	25.113	15.822		32.84		A
	ATOM	874	CB	SER	Α	176	23.938	26.155	16.901	1.00	33.54		Α
	ATOM	875	OG	SER	Α	176	22.599	26.056	17.347	1.00	34.86		Α
	ATOM	876	С	SER	Α	176	23.796	23.731	16.276	1.00	32.34		Α
	ATOM	877	Ō			176	22.726	23.263	15.884		32.82		Α
3 5		. 878	N			177	24.609	23.085	17.103		29.39		Α
22							24.313		17.597		27.20		A
	MOTA	879	CA			177		21.743					A
	, MOTA	880	CB			177	25.621	20.989	17.865		26.39		
	ATOM	881	CG			177	26.372	20.585	16.622		26.18		A
	ATOM	882	CD1	PHE	Α	177	26.210	21.277	15.426		25.30		A
40	ATOM	883	CD2	PHE	Α	177	27.266	19.516	16.662	1.00	26.05		Α
	ATOM	884	CEl	PHE	Α	177	26.923	20.912	14.290	1.00	26.59		Α
	MOTA	885		PHE			27.986	19.143	15.532	1.00	26.06		Α
	ATOM	886	CZ	PHE			27.815	19.841	14.343	1.00	25.42		A
		887	C	PHE			23.500	21.752	18.884		27.00		A
45	ATOM		_				23.704		19.747		26.48		A
45	ATOM	888	0	PHE									
	MOTA	889	N	ASP			22.578	20.802	19.022		26.70		A
	ATOM	890	CA	ASP			21.816	20.729	20.260		26.35		A
	ATOM	891	CB	ASP	Α	178	20.621	19.773	20.142	1.00	29.90		Α
	ATOM	892	CG	ASP	Α	178	21.020	18.372	19.720	1.00	32.28		Α
50	ATOM	893		ASP			22.157	17.949	20.014	1.00	35.21		A
	ATOM	894		ASP			20.179	17.683	19.105		34.79		Α
			C	ASP			22.810	20.228	21.311		25.03		A
	ATOM	895									21.24		Α.
	ATOM	896	0	ASP			23.974	19.968	20.992				
	MOTA	897	N	GLU			22.361	20.083	22.552		23.60		A
55	MOTA	898	CA	GLU			23.247	19.644	23.619		25.18	-	A
	MOTA	899	CB	GLU			22.542	19.770	24.971		27.60		Α
	ATOM	900	CG	GLU	Α	179	23.324	19.176	26,130	1.00	32.58		A ·
•	ATOM	901	CD	GLU			22.997	19.845	27.449	1.00	35.82	-	Α
	ATOM	902		GLU			21.825	20.224	27.645	1.00	35.95		A
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	ATOM	903	OE2	GLU	Α	179			23.912	19.984	28.291	1.00	38.19	A
	ATOM	904	С	GLU	Α	179			23.808	18.235,	23.450		24.08	Ā
	ATOM	905	0	GLU	A	179			24.977	17.989	23.756	1.00	22.79	A
	ATOM	906	N	THR	Α	180			22.983	17.316	22.961	1.00	23.36	A
5	ATOM	907	CA	THR	Α	180			23.412	15.935	22.761		22.15	A
	ATOM	908	СВ	THR	Α	180			22.224	15.054	22.320		23.77	A
	ATOM	909	OG1	THR	Α	180			21.222	15.075	23.341		26.37	A
	ATOM	910	CG2	THR	Α	180			22.670	13.616	22.088		22.66	A
	ATOM	911	С			180			24.533	15.830	21.724		22.01	A
10	ATOM	912	0	THR					25.533	15.141	21.944		19.87	A
	ATOM	913	N	CYS					24.365	16.511	20.596		21.21	A
	ATOM .	914	CA	CYS					25.372	16.480	19.541		22.22	A
	ATOM	915	CB	CYS					24.800	17.065	18.250		24.62	A
	ATOM .	916	SG	CYS					23.435	16.080	17.560		29.50	A
15	ATOM	917	c	CYS					26.633	17.232	19.954		23.07	A
~~	ATOM	918	Ö	CYS					27.746	16.827	19.608		23.95	A
	ATOM	919	N	THR					26.463	18.325	20.695		22.76	A
	ATOM	920	CA	THR					27.606	19.103	21.161		21.49	A
	ATOM	921	CB	THR					27.167	20.346	21.978		21.37	A
20	ATOM	922		THR					26.459	21.262	21.134		22.50	A
20	ATOM	923		THR					28.379	21.046	22.565		18.36	A
	ATOM	924	C	THR					28.454	18.215	22.071		21.48	A
	ATOM	925	Ö	THR					29.669	18.090	21.894		19.95	A
	ATOM	926	N	ARG					27.798	17.602	23.050		18.97	Ā
25	ATOM	927	CA	ARG					28.468	16.723	23.996		19.39	A
23	ATOM	928	CB	ARG					27.455	16.140	24.984		19.46	A
	ATOM	929	CG	ARG					28.030	15.062	25.887		18.77	A
	ATOM	930	CD	ARG					27.021	14.571	26.925		21.19	A
	ATOM	931	NE	ARG					26.605	15.642	27.824		19.46	A
30	ATOM	932	CZ	ARG					25.496	16.362	27.624		20.45	A
30	ATOM	933		ARG					24.672	16.123	26.666		19.81	A
	ATOM	933		ARG					25.224	17.338	28.539		17.11	A
	ATOM	935	C	ARG					29.206	15.577	23.302		20.02	A
	ATOM	936	Ö	ARG					30.383	15.333	23.573		19.97	A
35	ATOM	937	N	PHE					28.520	14.871	22.409		19.24	A
33							~		29.144	13.746	21.722		18.04	A
	ATOM ATOM	938 939	CA CB	PHE PHE					28.158	13.746	20.764		21.05	A
		940		PHE					28.719	11.857	20.704		22.67	A
	ATOM	941	CG	PHE					28.717	10.630	20.056		22.97	A
40	ATOM	941		PHE					29.317	11.949	18.850		19.97	A A
40	ATOM ATOM			PHE					29.317	9.510	20.176			
		943							29.308	10.833	18.263		23.53	A
	ATOM	944		PHE					29.915		18.928			A
	ATOM	945	CZ	PHE			-			9.613			22.97	A
15	ATOM.	946	C	PHE					30.403	14.127	20.941		17.99	A
45	ATOM	947	0	PHE					31.461	13.531	21.130		18.89	A
	ATOM	948	N	TYR					30.292	15.110	20.056		15.73	A
	ATOM	949	CA	TYR					31.443	15.519	19.265		15.72	A
	ATOM	950	CB	TYR					30.992	16.413	18.111		17.33	A
	ATOM	951	CG	TYR			-	-	30.364	15.584	17.015		19.37	A
50	ATOM	952		TYR					31.159	14.809	16.168		16.53	A
	ATOM	953		TYR					30.590	13.952	15.232		18.12	A
	ATOM	954		TYR					28.976	15.484	16.892		18.18	A
	ATOM	955		TYR					28.398	14.623	15.956		18.90	A
	ATOM	956	CZ	TYR					29.211	13.861	15.133		18:41	A
55	ATOM	957	ОН	TYR					28.650	12.995	14.218		20.48	A
	ATOM	958	С	TYR					32.544	16.172	20.083		15.79	A
	ATOM	959	0	TYR					33.720	16.015	19.766		17.69	A
	ATOM	960	N	THR					32.176	16.887	21.142		15.68	, A
	ATOM	961	CA	THR	А	186			33.184	17.504	21.997	1.00	16.03	A

	ATOM	962	CB	THR.	A 186		32.559	18.403	23.094	1.00 16.62	A
	ATOM	963	OG1		A 186	•	31.866	19.503	22.481	1.00 14.79	· A
		964	CG2		A 186		33.656	18.953	24.019	1.00 14.68	A
	ATOM				A 186		33.954	16.375	22.680	1.00 15.59	A
_	MOTA	965	С				35.176	16.443	22.823	1.00 13.77	A
5	ATOM	966	0		A 186			•			
	ATOM	.967	N		A 187		33.234	15.333	23.097	1.00 14.06	A
	ATOM	968	CA		A' 187		33.869	14.196	23.757	1.00 14.74	
	ATOM	969	CB	ALA	A 187		32.810	13.195	24.224	1.00 14.32	A
	ATOM	970	С	ALA	A 187		34.875	13.509		1.00 14.41	A
10	MOTA	971	0	ALA	A 187		35.972	13.136	23.247	1.00 15.61	A
	ATOM	972	N	GLU	A 188		34.516	13.340	21.549	1.00 14.01	A
	ATOM	973	CA		A 188		35.443	12.704	20.615	1.00 13.50	A
•	ATOM	974	CB		A 188	-	34.782	12.449	19.251	1.00 12.85	A
		975	CG		A 188		33.622	11.454	19.282	1.00 12.71	A
1.5	MOTA				A 188		33.464	10.685	17.979	1.00 15.01	A
15	MOTA	976	CD				33.404	11.275	16.899	1.00 13.21	A
	ATOM	977			A 188					1.00 17.69	A
	MOTA	978			A 188		33.110	9.484	18.031		A
	MOTA	979	С		A 188		36.682	13.582	20.436	1.00 13.34	
	MOTA	980	0		A 188		37.803	13.085	20.408	1.00 14.69	A
20	ATOM	981	N	ILE	A 189		36.486	14.893	20.326	1.00 13.52	A
	ATOM	982	CA	ILE	A 189		37.627	15.787	20.159	1.00 13.35	, A
	ATOM	983	CB	ILE	A 189		37.169	17.247	19.939	1.00 13.95	A
	ATOM	984	CG2	ILE	A 189		38.381	18.165	19.822	1.00 12.47	A
	ATOM	985			A 189		36.302	17.332	18.671	1.00 13.44	A
25	ATOM	986			A 189		35.588	18.664	18.491	1.00 14.29	A
23		987	C		A 189		38.530	15.702	21.394	1.00 14.63	A
	MOTA		0		A 189		39.753	15.595	21.271	1.00 12.97	A
	ATOM	988					37.927	15.751	22.582	1.00 14.35	A
	MOTA	989	N		A 190		38.684	15.655	23.832	1.00 13.22	A
	MOTA	990	CA		A 190				25.061	1.00 14.28	A
30	MOTA	991	CB		A 190		37.743	15.690	26.326	1.00 15.08	A
	MOTA	992			A 190		38.509	15.267		1.00 13.00	A
	ATOM	993	CG2		A 190		37.160	17.082	25.233		A
	MOTA	994	С		A 190		39.468	14.338	23.859	1.00 14.61	A
	MOTA	995	0	VAL	A 190		40.634	14.304	24.250	1.00 13.72	
35	ATOM .	996	N	SER	A 191		38.825	13.254	23.432	1.00 15.26	A
	MOTA	997	CA	SER	A 191		39.478	11.943	23.421	1.00 16.81	A
	ATOM	998	CB	SER	A 191		38.470	10.857	23.041	1.00 16.14	A
	ATOM	999	OG	SER	A 191		39.018	9.569	23.238	1.00 16.94	A
	ATOM	1000	C		A 191		40.649	11.928	22.441	1.00 16.58	A
40	ATOM	1001	ō		A 191		41.697	11.335	22.713	1.00 13.96	A
70	ATOM	1002	N		A 192		40.468	12.586	21.300	1.00 15.26	A
	ATOM	1002	CA		A 192		41.518	12.645	20.292	1.00 14.37	A
			CB		A 192		40.989	13.296	19.016	1.00 14.43	Α
	ATOM	1004			A 192		42.695	13.440	20.845	1.00 16.46	Α
	ATOM	1005	С				43.851	13.038	20.697	1.00 17.96	. A
45	ATOM	1006	0	ALA	A 192		42.401	14.563	21.496	1.00 15.02	A
	ATOM	1007	N		A 193						A
	MOTA	1008	CA		A 193		43.459	15.392	22.067		_
	ATOM	1009	CB		A 193		42.884	16.712	22.600		
	ATOM	1010	CG		A 193		42.445	17.721	21.525	1.00 15.97	A
٠50	ATOM	1011			A 193		41.869	18.979	22.190	1.00 13.97	A
	ATOM	1012	CD2		A 193		43.642	18.088	20.655	1.00 14.58	A
	MOTA	1013	С	LEU	A 193	}	44.211	14.659	23.174	1.00 14.49	A
	ATOM	1014	0		A 193		45.427	14.813	23.310	1.00 16.56	· , A
	ATOM	1015	N		A 194		43.500	13.870	23.975	1.00 13.96	A
55	ATOM	1016	CĄ		A 194		44.179	13.123	25.032	1.00 14.08	A
55	ATOM	1017	CB		A 194		43.190	12.295	25.857	1.00 14.65	A
	ATOM	1018	CG		A 194		43.882	11.301	26.789	1.00 17.09	Α
		1018	CD		A 194		42.924	10.592	27.730	1.00 19.59	A
	ATOM				A 194		41.809	10.237	27.295	1.00 19.25	Α
	MOTA	1020	OB.	اللق ا	A 194	•	41.005	20.201			

	ATOM	1021	OE2	GLU	A	194	43.302	10.380	28.906	1.00	20.20	Α
	ATOM	1022	С	GLU	Α	194	45.208	12.199	24.386	1.00	13.57	· A
	MOTA	1023	0	GLU	A	194	46.337	12.093	24.847	1.00	14.23	A
	MOTA	1024	N	TYR	Α	195·	44.822	11.544	23.301	1.00	14.89	A
5	ATOM	1025	CA	TYR	Α	195	45.743	10.642	22.618	1.00	16.58	Α
	ATOM	1026	CB	TYR	Α	195	45.030	9.910	21.488	1.00	17.29	Α
	ATOM	1027	CG	TYR			45.956	9.058	20.649		17.92	A
	ATOM	1028		TYR			46.347	7.788	21.077		17.96	A
	ATOM	1029		TYR			47.203	6.996	20.304		19.77	A
10	ATOM	1030	CD2				46.445	9.524	19.428		16.67	A
10	ATOM	1031	CE2	TYR			47.299	8.744	18.650		18.51	A
		1031	CZ	TYR			47.671	7.481	19.094		20.24	A
	ATOM	1032		TYR			48.506	6.705	18.325		21.89	A
	ATOM		ОН				46.917	11.419	22.035		16.98	A
1.5	ATOM	1034	С	TYR						-		
15	ATOM	1035	0	TYR			48.081	11.047	22.203		14.61	A
	ATOM	1036	N	LEU			46.599	12.507	21.347		16.30	A
	MOTA	1037	CA	LEU			47.619	13.328	20.720		18.15	A
	MOTA	1038	CB	LEU			46.969	14.502	19.982		18.59	A
	ATOM	1039	CG	LEU			47.834	15.203	18.935		22.51	A
20	ATOM	1040	CD1	LEU	A	196	48.222	14.206	17.841		20.94	$\mathbf{A}_{.}$
	MOTA	1041	CD2	LEU	A	196	47.060	16.375	18.338		22.98	A
	ATOM	1042	С	LEU	A	196	48.592	13.844	21.763	1.00	17.75	A
	MOTA	1043	0	LEU	A	196	49.801	13.644	21.649	1.00	18.33	A
	MOTA	1044	N	HIS	A	197	48.064	14.495	22.792	1.00	17.12	A
25	ATOM	1045	CA	HIS	Α	197	48.913	15.042	23.842	1.00	18.47	A
	ATOM	1046	CB	HIS	Α	197	48.069	15.866	24.817	1.00	15.90	A
	MOTA	1047	CG	HIS	Α	197	47.571	17.152	24.231	1.00	19.15	A
	ATOM	1048	CD2	HIS	A	197	47.830	17.745	23.038	1.00	18.22	A
	ATOM	1049	ND1	HIS	Α	197	46.704	17.992	24.897	1.00	17.47	A
30	ATOM	1050		HIS			46.450	19.047	24.139	1.00	19.74	A
50	ATOM	1051		HIS			47.119	18.921	23.007	1.00	15.69	A
	ATOM	1052	C	HIS			49.696	13.958	24.572		19.40	Α
	ATOM	1053	Ö	HIS			50.823	14.192	25.021		19.42	A
	ATOM	1054	N	GLY			49.106	12.770	24.679		18.59	A
35	ATOM	1055	CA	GLY			49.793	11.675	25.339		19.60	A
22		1056	C	GLY			51.075	11.307	24.612		21.86	A
	ATOM	1057	0	GLY			51.963	10.682	25.186		23.09	A
	ATOM	1057		LYS			51.174	11.687	23.341		22.81	A
	MOTA		N	LYS			52.368	11.401	22.549		24.43	A
40	ATOM	1059	CA	LYS			51.990	10.905	21.154		26.00	A
40	ATOM	1060	CB					9.520			30.98	A.
	ATOM	1061	CG	LYS			51.378		21.133 19.708		36.85	A
	ATOM	1062	CD	LYS			51.291	9.002			40.37	A
	ATOM	1063	CE	LYS .			50.832	7.559	19.682			
	MOTA	1064	ΝZ	LYS			51.646	6.691	20.581		43.48	A
45	ATOM	1065	C	LYS				12.631			23.88	A
	MOTA	1066	0	LYS			54.144	12.669	21.568		24.97	A
	ATOM	1067	И	GLY .			52.997	13.638	23.243		24.00	A
	MOTA	1068	CA	GLY			53.790	14.853	23.203		22.12	A
	ATOM	1069	С			200 ,	53.665	15.632	21.907		22.14	A·
50	ATOM	1070	0	GLY .	A	200	54.632	16.231	21.439		22.41	A
	ATOM	1071	N	ILE .			52.475	15.630	21.320		20.00	A
	MOTA	1072	CA	ILE .	Α	201	52.252	16.355	20.080		18.93	A
	ATOM	1073	CB	ILE .	A	201	51.784	15.414	18.955		19.70	A
	ATOM	1074		ILE .	Α	201	51.414	16.226	17.716	1.00	20.12	A
55	ATOM	1075	CG1	ILE .	Α	201	52.880	14.395	18.636	1.00	20.03	A
-	ATOM	1076		ILE .			52.408	13.258	17.745	1.00	22.75	Α
	ATOM	1077	C	ILE .			51.193	17.425	20.270		19.87	A
	ATOM	1078	ō	ILE			50.121	17.161	20.817		2Ò.08	A
	ATOM	1079	N	ILE			51.508	18.633	19.815		19.94	A

	ATOM	1080	CA	ILE	A 202	50.601	19.772	19.891	1.00 20.45	. А
	MOTA	1081	СВ	ILE	A 202		21.040	20.356	1.00 22.21	· A
	MOTA	1082	CG2	ILE .	A 202		22.220	20.470	1.00 22.67	A
•	ATOM	1083		L ILE			20.775	21.700	1.00 24.19	
5	ATOM	1084		LILE			21.920	22.169	1.00 24.19	A
•	ATOM	1085	C C		A 202		19.999	18.464		A
	ATOM	1086	o		A 202				1.00 20.71	A
							20.067	17.538	1.00 19.48	A
	ATOM	1087	N		A 203		20.108	18.270	1.00 18.65	Α
10	ATOM	1088	CA		A 203		20.319	16.919	1.00 18.02	A
10	ATOM	1089	CB		A 203		20.057	16.874	1.00 16.31	A
	ATOM	1090	CG		A 203		20.136	15.495	1.00 18.36	A
	ATOM	1091		HIS			21.186	14.655	1.00 16.42	. A
	MOTA	1092		. HIS			19.026	14.806	1.00 19.50	A
	MOTA	1093	CE1	. HIS 2	A 203	45.359	19.389	13.600	1.00 17.64	A
15	MOTA	1094	NE2	HIS	A 203	45.522	20.694	13.483	1.00 20.87	. А
	MOTA	1095	С	HIS Z	A 203	48.589	21.738	16.405	1.00 18.92	, A
	ATOM	1096	0	HIS 2	A 203		21.906	15.282	1.00 16.21	A
	ATOM	1097	N		A 204		22.744	17.232	1.00 18.60	A
	ATOM	1098	CA		A 204		24.157	16.914	1.00 19.81	A
20	ATOM	1099	СВ		A 204		24.365	16.458	1.00 19.81	
20	ATOM	1100	CG		A 204		24.303			A
	ATOM	1101	CD		A 204	• •		17.550	1.00 23.82	· A
	ATOM	1101					24.870	17.252	1.00 27.62	A
					A 204		24.449	15.994	1.00 29.43	A
0.5	ATOM	1103	CZ		A 204		24.861	15.572	1.00 33.10	A
25	ATOM	1104		ARG A			25.706	16:311	1.00 32.12	A
	MOTA	1105		ARG A			24.426	14.418	1.00 30.25	A
	ATOM	1106	С		A 204		24.830	15.905	1.00 20.03	Α
	MOTA	1107	0		A 204		26.038	15.698	1.00 20.88	Α
	ATOM	1108	N	ASP A	A 205	46.755	24.071	15.255	1.00 18.96	A
30	MOTA	1109	CA	ASP A	A 205	45.828	24.692	14.325	1.00 17.90	A
	ATOM	1110	CB	ASP A	A 205	46.418	24.741	12.914	1.00 18.95	A
	ATOM	1111	CG	ASP A	A 205	45.655	25.688	12.008	1.00 20.36	A
	ATOM	1112	OD1	ASP A	A 205	44.939	26.560	12.545	1.00 20.35	A
	ATOM	1113		ASP A			25.573	10.771	1.00 22.49	A
35	ATOM	1114	С	ASP A			23.956	14.328	1.00 19.60	A
	ATOM	1115	ō	ASP A		43.876	23.751	13.287	1.00 21.53	A
	ATOM	1116	N	LEU A			23.569	15.521	1.00 18.53	A
	ATOM	1117	CA	LEU F		42.813	22.851	15.667		
	ATOM	1118	CB	LEU F		42.693	22.295		1.00 19.18	A
40	ATOM	1119	•					17.087	1.00 18.94	A
40			CG	LEU A		41.511	21.358	17.346	1.00 23.10	A
	ATOM	1120		LEU A		41.615	20.142	16.436	1.00 23.01	A
	MOTA	1121	CD2			41.504	20.933	18.808	1.00 22.97	A
	ATOM	1122	c -	LEU A		41.639	23.772	15.361	1.00 19.05	A
	ATOM	1123	0	LEU A		41.556	24.880	15.886	1.00 19.25	A
45	ATOM	1124	N	LYS A		40.740	23.307	14.500	1.00 17.54	Α
	MOTA	1125	CA	LYS A		39.564	24.081	14.110	1.00 18.60	A
	MOTA	1126	CB	LYS A	207	39.980	25.248	13.196	1.00 18.98	Α
	MOTA	1127	CG	LYS A	207	40.786	24.817	11.982	1.00 18.20	Α
	MOTA	1128	CD	LYS A	207	41.246	26.000	11.139	1.00 21.42	Α
50	MOTA	1129	CE	LYS A	207	42.223	25.537	10.062	1.00 23.21	A
	ATOM	1130	ΝZ	LYS A	207	42.561	26.604	9.084	1.00 29.61	A
	ATOM	1131	C	LYS A		38.566	23.181	13.388	1.00 18.18	A
	ATOM	1132	O	LYS A		38.921	22.100	12.915	1.00 18.11	A
	ATOM	1133	N	PRO A		37.298	23.614	13.293	1.00 20.26	A
55	ATOM	1134	CD	PRO A		36.713	24.833	13.882	1.00 20.20	A
	ATOM	1135	CA	PRO A		36.272	22.814	12.616	1.00 18.79	A
	ATOM	1136	CB	PRO A		35.063				
	ATOM	1137	CG	PRO A		35.231	23.742	12.608	1.00 19.45	A
	ATOM	1137	C				24.509	13.891	1.00 21.81	A
	A1OE	TT-00		PRO A	. 200	36.674	22.372	11.209	1.00 21.04	A

			^	BB0	_	000		26 064	01 207	10 751	1.00 21.19		70
	MOTA	1139	0	PRO .		•		36.264	21.307	10.751			A
	ATOM	1140	N	GLU .				37.474	23.188	10.528	1.00 21.69		A
	MOTA	1141	CA	GLU .				37.928	22.872	9.170	1.00 22.64		A
	ATOM	1142	CB	GLU .	Α	209		38.644	24.084	8.558	1.00 23.65		A
5	ATOM	1143	CG	GLU .	Α	209		39.253	23.825	7.185	1.00 27.24		A
	ATOM	1144	CD	GLU :	Α	209		40.155	24.958	6.716	1.00 29.40		Α
	ATOM	1145	OE1	GLU .	Α	209		39.660	26.094	6.553	1.00 29.68		Α
•	ATOM	1146	OE2	GLU .	Z A	209		41.363	24.711	6.511	1.00 30.07		Α
		1147	C	GLU .				38.879	21.668	9.159	1.00 22.28		Α
10	ATOM			GLU .				38.955	20.933	8.170	1.00 21.36		A
10	ATOM	1148	0							10.263	1.00 19.90		A
	MOTA	1149	N	ASN .				39.600	21.490				A
	MOTA	1150	CA	ASN .				40.574	20.412	10.436	1.00 19.44		
	ATOM	1151	CB	ASN .				41.744	20.912	11.287	1.00 20.07		A
	ATOM	1152	CG	ASN .	A	210		42.746	21.698	10.479	1.00 25.77		A
15	ATOM	1153	OD1	ASN .	Α	210		43.571	22.427	11.029	1.00 26.73		Α
	ATOM	1154	ND2	ASN .	A	210		42.687	21.548	9.158	1.00 25.15		Α
	ATOM	1155	С	ASN .				40.005	19.151	11.078	1.00 18.63		Α
	ATOM	1156	Ö	ASN			•	40.712	18.154	11.234	1.00 18.29		Α
	ATOM	1157	N	ILE				38.739	19.202	11.469	1.00 16.31		Α
20				ILE				38.090	18.058	12.085	1.00 15.49		A
20	ATOM	1158	CA					37.336	18.488	13.354	1.00 15.40		Α
	ATOM	1159	CB	ILE .							1.00 13.40		A
	MOTA	1160		ILE				36.582	17.311	13.950			
	ATOM	1161		ILE				38.342	19.046	14.365	1.00 15.91		A
	MOTA	1162	CD1	ILE				37.720	19.669	15.590	1.00 15.98		A
25	ATOM	1163	С	ILE	Α	211	•	37.131	17.485	11.059	1.00 17.26		A
	ATOM	1164	0	ILE	Α	211		35.995	17.947	10.926	1.00 18.16		A
	ATOM	1165	N	LEU	Α	212		37.599	16.486	10.317	1.00 15.97		Α
	ATOM	1166	CA	LEU	Α	212		36.784	15.875	9.274	1.00 17.08		Α
	ATOM	1167	СВ	LEU				37.685	15.249	8.202	1.00 17.78		Α
30	MOTA	1168	CG	LEU				38.785	16.157	7.640	1.00 18.92		Α
30		1169		LEU				39.476	15.450	6.485	1.00 22.09		A
	ATOM							38.188	17.482	7.166	1.00 19.91		A
	ATOM	1170		LEU					14.825	9.837	1.00 18.35		A
	ATOM	1171	С	LEU				35.843			1.00 10.33		Α
	ATOM	1172	0	LEU				35.957	14.433	11.002			A
35	ATOM	1173	N	LEU				34.915	14.368	9.000	1.00 17.84		
	MOTA	1174	CA	LEU				33.942	13.362	9.403	1.00 19.94		A
	ATOM	1175	CB	LEU	A	213		32.556	14.004	9.487	1.00 20.84		A
	MOTA	1176	CG	LEU	Α	213		32.396	15.059	10.583	1.00 20.31		A
	ATOM	1177	CD1	LEU	Α	213		31.124	15.837	10.367	1.00 22.75		Α
40	ATOM	1178	CD2	LEU	A	213		32.379	14.378	11.940	1.00 23.93		Α
	ATOM	1179	C			213		33.914	12.187	8.426	1.00 20.98		Α
	ATOM	1180	Ö	LEU				33.743	12.379	7.218	1.00 19.55		Α
	ATOM	1181	N	ASN				34.088	10.970	8.935	1.00 20.44		A
		1182	CA	ASN				34.055	9.814	8.049	1.00 23.77		Α
4.5	ATOM							34.745			1.00 25.30		A
45	ATOM	1183		ASN							1.00 32.04		A
	ATOM	1184	CG.					34.077	8.127	9.948			
	MOTA	1185		ASN				32.908	8.422	10.206	1.00 34.43		A
	MOTA	1186	ND2	ASN				34.818	7.369	10.752	1.00 33.85		A
	ATOM	1187	С	ASN				32.618	9.466	7.693	1.00 24.07		A
50	ATOM	1188	0	ASN	Α	214		31.672	10.113	8.150	1.00 19.94		A
	ATOM	1189	N	GLU	Α	215		32.459	8.433	6.879	1.00 25.77		Α
	ATOM	1190	CA	GLU				31.138	8.003	6.445	. 1.00 28.69		Α
	ATOM	1191	CB	GLU				31.275	6.796	5.513	1.00 31.98		Α
	ATOM	1192	CG	GLU				29.970	6.334	4.896	1.00 40.22		Α
55	ATOM	1193	CD	GLU				30.182	5.312	3.795	1.00 44.27		Α
,,		1194		GLU				30.817	4.268	4.065	1.00 46.46		Α
	ATOM								5.556	2.660	1.00 46.13		A
	ATOM	1195		GLU				29.716			1.00 40.13	*	A
	MOTA	1196	C	GLU				30.188	7.673	7.601			
	ATOM	1197	0	GLU	A	215		28.971	7.769	7.447	1.00 28.52		A

	MOTA	1198	N	ASP	Α	216	-	30.7	137	7.287	8.752	1.00	26.77	A
	ATOM	1199	CA			216		29.9	14	6.953	9.91		27.28	A
	ATOM	1200	CB			216		30.5		5.795	10.696		31.27	A
	ATOM	1201	CG			216		30.3		4.466	9.979		37.61	A
5	ATOM	1202		ASP				29.2			9.499		39.45	A
•	ATOM	1203		ASP				31.3		3.710			41.84	
	ATOM	1203	C			216		29.6		8.135	10.862			A
	ATOM	1204	Ö			216		29.1		7.984			26.37	A
	ATOM	1205				217		30.1			11.950		25.73	A
10			N			217		30.1		9.306	10.441		23.02	A
10	ATOM	1207	CA							10.527	11.218		21.83	A
	MOTA	1208	CB			217		28.5		10.789	11.517		23.24	A
	ATOM	1209	CG			217		27.7		11.186	10.274		22.98	A
	MOTA	1210	SD			217		28.4		12.616	9.430		.27.57	A
	ATOM	1211	CE			217		27.6		13.974	10.332		26.68	A
15	ATOM	1212	С			217		30.8		10.618	12.502		21.51	Α
	ATOM	1213	0	MET	Α	217		30.4		11.323	13.440	1.00	18.62	Α
	ATOM	1214	N	HIS	Α	218		31.9	57	9.892	12.544	1.00	20.10	Α
	ATOM	1215	CA	HIS	Α	218		32.8	73	9.964	13.678	1.00	19.86	A
	ATOM	1216	CB	HIS	A	218		33.4	82	8.594	13.977	1.00	20.21	A
20	ATOM	1217	CG	HIS	Α	218		32.5	51	7.667	14.698	1.00	22.40	Α
	ATOM	1218	CD2	HIS	A	218		31.9	10	6.547	14.287	1.00	21.27	Α
	ATOM	1219	ND1	HIS	Α	218		32.1	77	7.863	16.011	1.00	19.59	Α
	MOTA	1220	CE1	HIS	Α	218		31.3	48	6.902	16.379	1.00	21.88	A
	ATOM	1221	NE2	HIS	Α	218		31.1	68	6.091	15.351	1,00	22.08	A
25	MOTA	1222	С	HIS	Α	218		33.9		10.921	13.172		19.10	A
	ATOM	1223	0	HIS				34.1		11.004	11.965		20.31	A
	ATOM	1224	N	ILE				34.6		11.638	14.067		17.21	A
	ATOM	1225	CA	ILE				35.6		12,586	13.618		15.26	A
	ATOM	1226	СВ	ILE				35.9		13.614	14.716		15.38	A
30	ATOM	1227		ILE				34.7		14.305	15.221		14.58	A
	ATOM	1228		ILE				36.7		12.919	15.864		14.46	A
	ATOM	1229		ILE				37.2		13.885	16.911		13.74	A
	ATOM	1230	C	ILE				36.9		11.944	13.161		16.21	A
	ATOM	1231	o	ILE				37.2		10.799	13.500		15.88	A
35	ATOM	1232	N	GLN				37.6		12.711	12.378		15.62	A
,	ATOM	1233	CA	GLN				38.9		12.711	11.876		17.84	A
	ATOM	1234	CB			220		38.8		11.595	10.525		20.00	A
	ATOM	1235	CG	GLN				38.4		10.129	10.659		26.97	A
	ATOM	1236	CD	GLN				38.6		9.343	9.372		29.95	A.
40	ATOM	1237		GLN				37.9		9.590	8.373		33.12	A
40	ATOM	1238	NE2	GLN							9.389			
		1239	C					39.5		8.393			30.47	A
	ATOM ATOM	1240	0	GLN GLN				39.7 39.6		13.610	11.735 10.751		17.00 18.27	A
	ATOM	1241	N					40.5		14.339	12.746			A
15				ILE						13.906			14.34	A
45	ATOM	1242	CA	ILE				41.3		15.120	12.753		14.46	A
	MOTA	1243	CB	ILE				41.8		15.416	14.175		12.30	A
	ATOM	1244		ILE				42.7		16.656	14.167		.14.78	A
	ATOM ·			ILE				40.6		15.613	15.102		13.92	A
	ATOM	1246		ILE				41.0		15.901	16.543		15.06	A
50	ATOM	1247	С	ILE				42.5		14.996	11.783		15.44	A
	ATOM	1248	0	ILE				43.1		13.915	11.613		13.93	A
	MOTA	1249	N	THR				42.8		16.101	11.127		15.36	A
	MOTA	1250	CA	THR				43.9		16.098	10.174		17.52	A
·-	ATOM	1251	CB	THR		-		43.4		15.836	8.750		19.92	A
55	ATOM	1252	0G1					44.5		15.637	7.875		18.78	A
	ATOM	1253	CG2					42.63	30	17.018	8.257		18.16	A
	MOTA	1254	С	THR				44.7		17.428	10.192		19.60	A
	MOTA	1255	0	THR				44.50		18.257	11.084		18.59	A
	ATOM	1256	N	ASP	Α	223		45.63	30	17.610	9.216	1.00	18.69	A

	. ATOM	1257	CA	ASP A	223	46.44	0 18.825	9.069	1.00 2	20.12	A
	ATOM	1258	CB	ASP A	223	45.53	20.065	9.108	1.00		A
	ATOM	1259	CG	ASP A		46.24		8.670	1.00		
	ATOM	1260				47.28					A
_				ASP A				7.975	1.00 2		A
5	ATOM	1261		ASP A		45.76		9.009	1.00 2		A
	MOTA	1262	C -	ASP A		47.51		10.150	1.00 2		Α
	ATOM	1263	0	ASP A	223	47.43	9 19.751	11.055	1.00 2	22.76	. A
	ATOM	1264	N	PHE A	224	48.53	5 18.063	10.027	1.00 2	20.75	A
	MOTA	1265	CA	PHE A		49.61		11.009	1.00 2		A
10	ATOM	1266	СВ	PHE A		49.80		11.424	1.00 2		A
10	ATOM	1267	CG	PHE A		48.68		12.263	1.00 2		
											A
	MOTA	1268		PHE A		48.59		13.614	1.00 2		A
	MOTA	1269		PHE A		47.68		11.693	1.00 2	22.27	A
	ATOM	1270	CE1	PHE A	224	47.52	8 15.868	14.389	1.00 2	23.30	A
15	ATOM	1271	CE2	PHE A	224	46.60	6 14.763	12.457	1.00 2	21.11	Α
	MOTA	1272	CZ	PHE A	224	46.53	0 15.093	13.807	1.00 2	22.02	. A
	ATOM	1273	C	PHE A		50.95		10.619	1.00 2		A
		1274	Õ	PHE A		51.90		11.407			
	ATOM								1.00 2		A
	ATOM	1275	N	GLY A		51.04		9.412	1.00 2		A
20	MOTA	1276	CA	GLY A		52.30		8.981	1.00 2		A
	ATOM	1277	С	GLY A	225	52.74	2 20.822	9.920	1.00 2	24.99	A
	MOTA	1278	0	GLY A	225	53.93	9 21.041	10.122	1.00 2	24.52	A
	ATOM	1279	N	THR A	226	51.77	9 21.524	.10.508	1.00 2	23.50	A
	ATOM	1280	CA	THR A		52.10		11.416	1.00 2		A
25	ATOM	1281	CB	THR A		51.19		11.160	1.00 2		A
23				THR A				11.113	1.00 2		A
	ATOM	1282									
	ATOM	1283		THR A		51.57		9.834	1.00 2		Α.
	MOTA	1284	С	THR A		52.04		12.894	1.00 2		A
	ATOM	1285	0	THR A	226	52.01	9 23.100	13.768	1.00 2	24.54	A
30	ATOM	1286	N	ALA A	227	52.03	7 20.935	13.173	1.00 2	24.97	Α
	ATOM	1287	CA	ALA A	227	52.00	4 20.475	14.550	1.00 2	25.49	A
	ATOM	1288	CB	ALA A	227	51.65	9 18.993	14.607	1.00 2	22.85	Α
	ATOM	1289	C	ALA A		53.38		15.149	1.00 2		. A
	ATOM	1290	Ö	ALA A		54.33		14.435	1.00 2		A
25									1.00 2		A
35	ATOM	1291	N	LYS A		53.49		16.461			
	MOTA	1292	CA	LYS A		54.76		17.149	1.00 3		A
	MOTA	1293	СВ	LYS A		54.69		18.054	1.00 3		A
	ATOM	1294	CG	LYS A	228	56.00	7 22.294	18.765	1.00 4	11.23	A
	ATOM	1295	CD	LYS A	228	57.08	2 22.725	17.768	1.00 4	17.57	A
40	ATOM	1296	CE	LYS A	228	58.40	1 23.056	18.462	1.00 4	19.82	A
	MOTA	1297	NZ	LYS A		59.45	9 23.425	17.480	1.00 5	1.49	· A
	ATOM	1298	C	LYS A		55.01			1.00 3		Α
	ATOM	1299		LYS A		54.19		18.815	1.00 3		A
		1300		VAL A		56.15		17.756			A
4.5	ATOM		N								
45	ATOM	1301	CA	VAL A		56.51		18.501	1.00 3		A
	MOTA	1302	CB	VAL A		57.24		17.609	1.00 3		A
	MOTA	1303	CG1	VAL A	229	57.61	9 15.419	18.415	1.00 3	32.34	A
	ATOM	1304	CG2	VAL A	229	56.37	0 16.264	16.436	1.00 3	34.25	A
	ATOM	1305	С	VAL A	229	57.42	0 18.035	19.668	1.00 3	37:57	A
50	ATOM	1306	0	VAL A		58.58		19.474	1.00 3		Α
••	ATOM	1307	N	LEU A		56.87		20.878	1.00 4		A
						57.61			1.00 4		A
	ATOM	1308	CA	LEU A				22.088			
	ATOM	1309	CB	LEU A		56.65		23.270	1.00 4		A
	ATOM	1310	CG	LEU A		55.62		23.207	1.00 4		Α
55	ATOM	1311	CD1	LEU A	230	54.67	3 19.430	24.383	1.00 4		A
	ATOM	1312	CD2	LEU A	230	56.34	0 20.885	23.214	1.00 4	4.81	A
	ATOM	1313	С	LEU A		58.69	5 17.279	22.440	1.00 5	0.42	A
	ATOM	1314	Ö	LEU A		58.60		22.089	1.00 5		A
	ATOM	1315	N	SER A		59.71		23.145	1.00 5		A

	A TOM	1316	CA	SER	71	231		60.824	16.914	23.583	1.00 61.14	70
•	ATOM ATOM	1317	CB	SER				62.077	17.200	22.750	1.00 61.14	A A
										22.730		
	ATOM	1318	OG	SER				62.444	18.568	25.071	1.00 62.85	A
_	ATOM	1319	С	SER					,17.126		1.00 64.65	A
5	ATOM	1320	0	SER				61.392	16.164	25.794	1.00 65.70	A
	MOTA	1321	N	PRO				61.081	18.387	25.549	1.00 67.54	A
	MOTA	1322	CD	PRO				60.854	19.651	24.823	1.00 68.60	A
	ATOM	1323	CA	PRO				61.358	18.655	26.966	1.00 68.74	A
	ATOM	1324	CB	PRO	A	232		61.109	20.158	27.086	1.00 68.83	A
10	ATOM	1325	CG	PRO	A	232		61.505	20.666	25.737	1.00 68.96	A
	MOTA	1326	С	PRO	Α	232		60.460	17.846	27.899	1.00 69.17	A
	ATOM	1327	0	PRO	A	232		59.335	17.494	27.541	1.00 69.94	Α
	ATOM	1328	N	ALA	Α	237		57.424	23.198	27.637	1.00 80.06	Α
	ATOM	1329	CA	ALA	Α	237		56.783	23.047	26.335	1.00 79.29	A
15	MOTA	1330	CB	ALA	Α	237		55.275	22.907	26.512	1.00 78.64	A
	MOTA	1331	c´	ALA	A	237		57.092	24.239	25.433	1.00 79.07	A
	ATOM	1332	0	ALA	Α	237		56.250	25.113	25.249	1.00 79.47	Α
	MOTA	1333	N	ALA	Α	238		58.297	24.280	24.871	1.00 78.57	A
	ATOM	1334	CA	ALA				58.683	25.383	23.992	1.00 78.50	А
20	MOTA	1335.	CB	ALA				60.186	25.347	23.728	1.00 78.50	A
	ATOM	1336	C	ALA				57.920	25.327	22.673	1.00 78.15	A
	ATOM	1337	Ō	ALA			•	57.243	24.341	22.375	1.00 77.96	A
	ATOM	1338	N	ALA				58.027	26.393	21.887	1.00 77.28	A
	ATOM	1339	CA	ALA		,		57.338	26.452	20.603	1.00 76.27	A
25	ATOM	1340	CB	ALA				55.849	26.489	20.827	1.00 76.61	A
23	ATOM	1341	C	ALA				57.766	27.667	19.793	1.00 75.38	A
	ATOM	1341	Õ	ALA				58.955	27.955	19.700	1.00 75.89	A
	ATOM	1343	N	ASN				56.781	28.357	19.700	1.00 73.85	A
				ASN				56.967	29.553	18.389	1.00 73.93	
20	ATOM	1344	CA	,								A
30	ATOM	1345	CB	ASN				58.151	30.400	18.874	1.00 71.47	A
	ATOM	1346	CG	ASN				59.459	30.055	18.174	1.00 72.06	A
	ATOM	1347		ASN				59.575	30.149	16.943	1.00 72.03	A
	ATOM	1348		ASN				60.470	29.665	18.964	1.00 71.91	A
0.5	ATOM	1349	C	ASN				57.188	29.178	16.928	1.00 69.41	A
35	ATOM	1350	0	ASN				57.480	28.024	16.624	1.00 70.09	A
	ATOM	1351	N	ALA				57.055	30.165	16.038	1.00 66.62	A
	ATOM	1352	CA	ALA				57.246	30.013	14.585	1.00 63.94	A
	MOTA	1353	С	ALA				55.952	30.080	13.772	1.00 60.63	Α
	ATOM	1354	0	ALA				55.840	30.880	12.845	1.00 61.29	Α
40	ATOM	1355	CB	ALA				57.979	28.704	14.246	1.00 65.23	A
	MOTA	1356	N	PHE				54.984	29.236	14.113	1.00 56.72	A
	ATOM	1357	CA	PHE				53.712	29.196	13.394	1.00 52.53	A
	ATOM	1358	CB	PHE				53.419	27.767	12.923	1.00 49.14	A
	ATOM	1359	CG	PHE				52.040	27.590	12.354	1.00 47.38	A
45	ATOM	1360		PHE				51.731	28.067		1.00 47.69	A
	ATOM	1361	CD2	PHE	A	242		51.038	26.975	13.102	1.00 45.45	A
	ATOM	1362	CE1	PHE	A	242		50:445	27.937	10.565	1.00 46.75	A
	ATOM	1363	CE2	PHE	Α	242		49.751	26.840	12.594	1.00 45.41	А
	ATOM	1364	cz	PHE	A	242	•	49.453	27.323	11.322	1.00 46.55	A
50	ATOM	1365	С	PHE.	A	242		52.534	29.688	14.229	1.00 50.08	A
	ATOM	1366	O	PHE .	Α	242		52.502	29.505	15.444	1.00 49.86	A
	ATOM	1367	N	VAL .	Α	243		51.566	30.305	13.557	1.00 47.67	A
	ATOM	1368	CA	VAL .	Α	243		50.355	30.809	14.200	1.00 46.21	A
	ATOM	1369	СВ	VAL .	Α	243		50.340	32.352	14.258	1.00 47.36	· A
55	ATOM	1370		VAL .	Α	243		49.012	32.844	14.825	1.00 47.54	A
	ATOM	1371		VAL .				51.497	32.842	15.109	1.00 48.50	A
	ATOM	1372	С	VAL .				49.150	30.342	13.389	1.00 44.12	· А
	ATOM	1373	0	VAL				48.956	30.765	12.247	1.00 44.46	A
	ATOM	1374	N	GLY .				48.348	29.467	13.985	1.00 40.48	· A

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	MOTA	1375	CA	GLY A	244	47.	176 2	8.941	13.306	1.00	37.65	A
•	MOTA	1376	С	GLY A	244	46.	101 2	9.960	12.964	1.00	35.39	A
	MOTA	1377	0	GLY A	244	46.	313 3	1.168	13.065	1.00	35.92	A
	ATOM	1378	N	THR A	245	44.	936 2	9.463	12.560	1.00	33.30	A
5	MOTA	1379	CA	THR A	245	43.	813 3	0.312	12.184	1.00	30.20	A
	MOTA	1380	CB	THR A	245	42.	593 2	9.450	11.829	1.00	32.00	A
	ATOM	1381	OG1	THR A	245	42.	952 2	8.573	10.755	1.00	32.81	A
	ATOM	1382	CG2	THR A	245	41.		0.319	11.390	1.00	28.34	A
	ATOM	1383	С	THR A		43.		1.296	13.296	1.00	27.96	A
10	ATOM	1384	Ō	THR A		43.		0.907	14.434		25,46	A
	ATOM	1385	Ń	ALA A		43.		2.576	12.938		25.22	A
	ATOM	1386	CA	ALA A		43.		3.675	13.867		23.27	A
	ATOM	1387	CB	ALA A		42.		4.955	13.082		22.94	А
	ATOM	1388	C	ALA A		42.		3.475	14.934		21.27	A
15	ATOM	1389	0	ALA A		42.		3.705	16.114		20.93	A
13		1390·	N	GLN A		40.		3.703	14.536		19.67	A
	ATOM	1391	CA	GLN A		39.		2.886	15.504		20.17	A
	ATOM	1391	CB	GLN A		38.		2.535	14.779		21.89	A
	ATOM					38.		3.076	13.355		26.18	A
00	ATOM	1393	CG	GLN A		37.		3.794	13.064		27.30	A
20	ATOM	1394	CD								30.13	A
	MOTA	1395	OE1	GLN A		36.		3.447	13.605		28.70	A
	MOTA	1396	NE2	GLN A		37.		4.792	12.189		19.43	A A
	MOTA	1397	C	GLN A		40.		1.849	16.595		18.93	A
	MOTA	1398	0	GLN A		39.		1.883	17.648			
25	ATOM	1399	N	TYR A		41.		0.948	16.359		18.60	A
	ATOM	1400	CA '	TYR A		41.		9.896	17.329		19,20	A
	MOTA	1401	CB	TYR A		41.		8.529	16.642		17.53	A
	MOTA	1402	CG	TYR A		40.		8.362	15.927		19.32	A
	ATOM	1403		TYR A		38.		8.010	16.625		17.69	A
30	MOTA	1404	CE1			37.		7.976	15.990		18.18	' A
	MOTA	1405	CD2	TYR A		. 39.		8.664	14.569		16.87	A
	ATOM	1406	CE2			38.		8.635	13.924		19.17	A
	ATOM	1407	CZ	TYR A	248	37.		8.295	14.643		19.46	Α
	MOTA	1408	OH	TYR A		36.		8.311	14.023		18.98	A
35	MOTA	1409	С	TYR A	. 248	42.		0.039	17.993		20.42	A
	MOTA	1410	0	TYR A	. 248	43.		9.191	18.792		19.19	A
	MOTA	1411	N	VAL A	249	43.		1.114	17.673		20.20	Α
	MOTA	1412	CA	VAL A	249	44.	841 3	1.343	18.251		20.91	Α
	MOTA	1413	СВ	VAL A	249	45.		2.532	17.570		21.18	A
40	ATOM	1414	CG1	VAL A	249	46.		2.896	18.317		22.45	A
	MOTA	1415	CG2	VAL A	249	45.		2.170	16.139		24.01	A
	ATOM	1416	С	VAL A	249	44.		1.606	19.750		21.52	A
	ATOM	1417	0	VAL A	249	43.		2.368	20.216		22.72	Α
	ATOM	1418	N	SER A	250	45.		0.965	20.503		20.70	A
45	ATOM	1419	CA	SER A	250	45.	697 3	1.133	21.951		21.65	A
	ATOM	1420	CB	SER A	250	46.	370 2	9.919	22.613		22.02	A
	ATOM	1421	OG	SER A	250	47.	692 2	9.725	22.132	1.00	22.12	A
	ATOM	1422	С	SER A	250	46.	476 3	2.402	22.280	1.00	22.13	Α
	ATOM	1423	0	SER A	250	47.	332 3	2.828	21.511	1.00	22.77	A
50	ATOM	1424	N	PRO P	251	46.	180 3	3.029	23.425	1.00	22.23	A
	MOTA	1425	CD	PRO A		45.	163 3	2.684	24.433	1.00	22.97	A
	ATOM	1426	CA	PRO P				4.254	23.800	1.00	22.52	Α
	ATOM	1427	CB	PRO P		46.		4.650	25.127	1.00	23.06	A
	ATOM	1428	CG	PRO A		45.		3.329	25.676	1.00	22.55	A
55	ATOM	1429	C	PRO A		48.		4.115	23.907		22.15	Α
	ATOM	1430	ō	PRO A		49.		5.047	23.563		22.62	, A
	ATOM	1431	N	GLU A		48.		2.966	24.367		20.69	A
	ATOM	1432	CA	GLU A		50.		2.772	24.500		21.40	A
	ATOM	1433	CB	GLU A		50.		1.382	25.071		20.59	A
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	MOTA	1434	CG	GLU	A	252	49.993	30.232	24.352	1.00 2	1.91	A
	ATOM	1435	CĎ	GLU	A	252	48.691	29.822	25.014	1.00 2	1.51	A
	ATOM	1436	OE1	GLU	Α	252	47.989	30.707	25.550	1.00 2	1.46	A
	ATOM	1437	OE2	GLU			48.367	28.613	24.993	1.00 2	0.23	· A
5	MOTA	1438	C	GLU			51.071	32.970	23.167	1.00 2	2.99	, A
	ATOM	1439	0	GLU	A	252	52.191	33.480	23.136	1.00 2	3.17	A
	ATOM	1440	N	LEU			50.441	32.576	22.064	1.00 2	3.00	Α
	ATOM	1441	CA	LEU	A	253	51.068	32.753	20.758	1.00 2	5.62	A
	ATOM	1442	CB	LEU	Α	253	50.277	32.029	19.669	1.00 2	6.75	A
10	MOTA	1443	CG	LEU	А	253	50.743	30.620	19.296	1.00 3	1.87	A
	MOTA	1444	CD1	LEU	Α	253	50.433	29.651	20.422	1.00 3	1.81	A
	MOTA	1445	CD2	LEU	A	253	50.044	30.179	18.015	1.00 3	1.86	A
	ATOM	1446	C	LEU	A	253	51.201	34.228	20.371	1.00 2	6.94	· A
	MOTA	1447	0	LEU	Α	253	52.107	34.601	19.626	1.00 2	7.09	A
15	ATOM	1448	N	LEU	A	254	50.297	35.059	20.877	1.00 2	5.83	A
	MOTA	1449	CA	LEU	Α	254	50.297	36.485	20.564	1.00 2	7.26	A
	MOTA	1450	CB	LEU	Α	254	48.858	37.006	20.564	1.00 2	5.84	A
	MOTA	1451	CG	LEU	Α	254	47.882	36.290	19.621	1.00 2	4.69	A
	ATOM	1452	CD1	LEU	Α	254	46.459	36.724	19.932	1.00 2	3.64	A
20	ATOM	1453	CD2	LEU	Α	254	48.236	36.597	18.177	1.00 2	4.24	A
	ATOM	1454	С	LEU	Α	254	51.134	37.314	21.537	1.00 3	0.62	А
	ATOM	1455	0	LEU	Α	254	51.633	38.383	21.187	1.00 3	2.35	· А
	ATOM	1456	N	THR-	Α	255	51.292	36.821	22.758	1.00 3	2.47	A
	MOTA	1457	CA	THR	Α	255	52.056	37.547	23.759	1.00 3	6.70	A
25	MOTA	1458	CB	THR	Α	255	51.368	37.478	25.127	1.00 3	4.51	A
	MOTA	1459	OG1	THR	Α	255	51.188	36.106	25.494	1.00 3	5.49	A
	ATOM	1460	CG2	THR	Α	255	50.013	38.166	25.077	1.00 3	3.40	A
	MOTA	1461	С	THR	Α	255	53.477	37.035	23.910	1.00 4	0.09	A
	MOTA	1462	0	THR	Α	255	54.430	37.793	23.772	1.00 4	3.69	A
30	MOTA	1463	N	GLU	Α	256	53.617	35.747	24.189	1.00 4	4.77	A
	MOTA	1464	CA	GLU	Α	256	54.932	35.144	24.382	1.00 4	9.15	A
	MOTA	1465	СВ	GLU	Α	256	54.866	34.143	25.534	1.00 5	1.24	-A
	ATOM	1466	CG	GLU	Α	256.	54.514°	34.786	26.862	1.00 5	6.03	A
	MOTA	1467	CD	GLU	Α	256	54.053	33.780	27.893	1.00 5	8.83	A
35	MOTA	1468	OE1	GLU	Α	256	54.766	32.776	28.107	1.00 6	2.13	A
	MOTA	1469	OE2	GLU	Α	256	52.979	33.996	28.494	1.00 6	0.34	A
	ATOM	1470	С	GLU	Α	256	55.475	34.456	23.137	1.00 5	0.09	A
	ATOM	1471	0	GLU	Α	256	56.616	33.995	23.127	1.00 5	0.42	A
	ATOM	1472	N	LYS	Α	257	54.658	34.389	22.090	1.00 5	1.21	A
40	MOTA	1473	CA	LYS	Α	257	55.064	33.746	20.845	1.00 5	1.22	A
	ATOM	1474	CB	LYS	Α	257	56.244	34.502	20.227	1.00 5	3.28	A
	ATOM	1475	CG	LYS	Α	257	56.558	34.125	18.790	1.00 5	5.19	A
	ATOM	1476	CĐ	LYS	A	257	57.709	34.961	18.253	1.00 5	7.52	A
	ATOM	1477	CE	LYS	Α	257	57.952	34.694	16.777	1.00 5	8.52	A
45	ATOM	1478	NZ	LYS	Α	257	58.290	33.268	16.515	1.00 6	0.88	A
	ATOM	1479	С	LYS			55.467	32.302	21.138	1.00 5	0.74	A
	ATOM	1480	0	LYS	A	257 [°]	56.432	31.790	20.577	1.00 5	2.26	· A
	MOTA	1481	N	SER			54.721	31.654	22.027	1.00 4	8.07	A
	ATOM	1482	CA	SER	Α	258	54.999	30.273	22.402	1.00 4	6.87	A
50	ATOM	1483	CB	SER	A	258	55.590	30.229	23.812	1.00 4	8.88	A
	ATOM	1484	OG	SER	Α	258	54.741	30.892	24.734	1.00 5	3.14	A
	ATOM	1485	С	SER	A	258	53.735	29.415	22.342	1.00 4	4.07	A
	ATOM	1486	0	SER			52.617	29.932	22.417	1.00 4	4.17	A
	ATOM	1487	N	ALA			53.917	28.105	22.204	1.00 3	8.30	A
55	ATOM	1488	CA	ALA			52.793	27.180	22.127	1.00 3	4.73	A
	ATOM	1489	CB	ALA	A	259	52.551	26.779	20.684	1.00 3		A
	ATOM	1490	С	ALA			53.042	25.940	22.977	1.00 3	2.34	A
	ATOM	1491	0	ALA			54.172	25.459	23.086	1.00 3	1.81	A
	ATOM	1492	N	CYS			51.975	25.428	23.579	1.00 2	8.58	A
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	ATOM	1493	CA	CYS .	A 260		52.056	24.244	24.425	1.00 26.27	A
	MOTA	1494	СВ	CYS .	A 260		52.183	24.654	25.892	1.00 26.53	Α.
	MOTA	1495	SG	CYS .	A 260		50.846	25.739	26.469	1.00 32.91	Α
	ATOM	1496	С	CYS .	A 260		50.786	23.435	24.224	1.00 22.83	A
5	ATOM	1497	0	CYS .	A 260		49.892	23.856	23.495	1.00 22.14	A
	MOTA	1498	N	LYS .	A 261		50.706	22.277	24.868	1.00 20.02	A
	ATOM	1499	CA	LYS .	A 261		49.526	21.434	24.744	1.00 20.65	A
	ATOM	1500	CB	LYS :	A 261	•	49:619	20.243	25.696	1.00 23.28	A
	ATOM	1501	CG	LYS !	A 261		50.716	19.253	25.347	1.00 27.44	A
10	ATOM	1502	CD	LYS :	A 261		50.732	18.117	26.350	1.00 29.98	· A
	ATOM	1503	CE	LYS	A 261		51.922	17.203	26.134	1.00 32.34	Α
	ATOM	1504	NZ		A 261		51.940	16.121	27.153	1.00 33.28	A
	ATOM	1505	C		A 261		48.268	22.229	25.062	1.00 19.20	A
	ATOM	1506	ō		A 261		47.253	22.092	24.387	1.00 18.08	A
15	ATOM	1507	N		A 262		48.358	23.068	26.089	1.00 16.92	Α
13	ATOM	1508	CA		A 262		47.235	23.883	26.534	1.00 18.13	Α
	ATOM	1509	CB		A 262		47.644	24.698	27.770	1.00 18.27	A
	ATOM	1510	OG		A 262		46.517	25.258	28.421	1.00 22.53	A
	ATOM	1511	C		A 262		46.736	24.811	25.424	1.00 16.77	Α
20	ATOM	1512	ō		A 262		45.591	25.254	25.450		. A
20	ATOM	1513	N		A 263		47.595	25.118	24.456	1.00 16.44	A
	ATOM	1514	CA		A 263		47.175	25.970	23.347	1.00 16.89	A
	ATOM	1515	CB		A 263		48.340	26.228	22.382	1.00 18.49	A
	ATOM	1516	OG		A 263		49.402	26.909	23.031	1.00 22.10	A
25	ATOM-	1517	C		A 263		46.040	25.257	22.612	1.00 17.79	A
23	ATOM	1518	o		A 263		45.099	25.898	22.148	1.00 17.57	Α
	ATOM	1519	N		A 264		46.119	23.928	22.517	1.00 16.30	A
	ATOM	1520	CA		A 264		45.069	23.166	21.836	1.00 16.72	A
	MOTA	1521	CB		A 264		45.483	21.704	21.620	1.00 15.92	. А
30	ATOM	1522	CG		A 264		46.544	21.539	20.548	1.00 17.93	A
50	ATOM	1523			A 264		46.642	22.412	19.661	1.00 16.78	A
	ATOM	1524			A 264		47.265	20.515	20.579	1.00 16.64	A
	ATOM	1525	C.		A 264		43.773	23.194	22.646	1.00 17.67	A
	ATOM	1526	Ö		A 264		42.681	23.197	22.076	1.00 18.27	A
35	ATOM	1527	N		A 265		43.898	23.205	23.974	1.00 15.49	A
33	ATOM	1528	CA		A 265		42.730	23.232	24.849	1.00 14.75	A
	ATOM	1529	СВ		A 265		43.147	23.038	26.313	1.00 11.38	A
	ATOM	1530	CG		A 265		43.711	21.641	26.621	1.00 14.04	A
	ATOM	1531			A 265		44.249	21.579	28.052	1.00 13.96	. A
- 40	ATOM	1532			A 265		42.619	20.603	26.416	1.00 11.62	A
	ATOM	1533	C		A 265		41.999	24.557	24.675	1.00 15.13	A
	ATOM	1534	Ö		A 265		40.777	24.620	24.785	1.00 16.75	A
	ATOM	1535	Ŋ		A 266		42.746	25.622	24.405	1.00 16.08	Α
	ATOM	1536	CA		A 266		42.118	26.918	24.184	1.00 16.96	A
45	ATOM	1537	СВ		A 266		43.176	28.015	24.023	1.00 17.28	A
73	ATOM	1538	CG		A 266		42.618	29.326	23.521	1.00 20.54	A
	ATOM	1539.			A 266		42.313	30.490	24.301	1.00 20.07	А
	ATOM	1540			A 266		41.782	31.459	23.417	1.00 20.46	A
	ATOM	1541			A 266		42.435	30.810	25.660	1.00 20.68	A
50	ATOM	1542			A 266		42.270	29.631	22.231	1.00 19.53	A
50	ATOM	1543			A 266		41.769	30.908	22.163	1.00 19.61	A
	ATOM	1544			A 266		41.372	32.727	23.850	1.00 20.90	A
	ATOM	1545			A 266		42.026	32.073	26.091 [.]	1.00 19.45	A
	ATOM	1546			A 266		41.501	33.015	25.185	1.00 20.71	A
55	MOTA	1547	C		A 266		41.284	26.795	22.913	1.00 17.22	A
55	ATOM	1548	ŏ		A 266		40.139	27.240	22.863	1.00 18.03	A
	ATOM	1549	N		A 267		41.863	26.181	21.886	1.00 17.50	A
	ATOM	1550	CA		A 267		41.155	25.990	20.626	1.00 16.16	A
	ATOM	1551	CB		A 267		42.050	25.290	19.621	1.00 14.28	A
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	ATOM	1552	С	ALA A	267	39.901	25.159	20.891	1.00 16.28	A
	ATOM	1553	0	ALA A	267	38.835	25.436	20.346	1.00 16.46	A
	ATOM	1554	N	LEU A	268	40.031	24.144	21.739	1.00 16.57	A
	ATOM	1555	CA	LEU A	268	38.890	23.299	22.084	1.00 17.03	A
5	ATOM	1556	CB	LEU A	268	39.292	22.260	23.139	1.00 15.35	A
	ATOM	1557	CG	LEU A		38.158	21.429	23.754	1.00 19.00	A
	ATOM	1558		LEU A		37.505	20.578	22.678	1.00 16.17	A
	ATOM	1559	CD2			38.718	20.537	24.881	1.00 17.49	A
	ATOM	1560	C	LEU A		37.766	24.179	22.628	1.00 15.72	· A
10	ATOM	1561	ŏ	LEU A		36.603	24.031	22.247	1.00 15.28	A
10	ATOM	1562	N	GLY A		38.119	25.099	23.520	1.00 14.34	A
	ATOM	1563	CA	GLY A		37.124	25.989	24.092	1.00 13.39	A
	ATOM	1564	C	GLY A		36.406	26.808	23.031	1.00 14.94	A
	ATOM	1565	0	GLY A		35.193	27.014	23.114	1.00 14.76	A
15	ATOM	1566	N	CYS A		37.146	27.279	22.030	1.00 13.86	A
13		1567	CA	CYS A		36.539	28.061	20.958	1.00 16.80	A
	MOTA	1568	CB	CYS A		37.611	28.634	20.023	1.00 15.00	A
	MOTA	1569	SG	CYS A		38.751	29.810	20.780	1.00 13.37	A
	ATOM	1570	C	CYS A		35.598	27.175	20.760	1.00 20.40	A
20	ATOM			CYS A		34.516	27.173	19.741	1.00 17.30	A
20	ATOM	1571	0					19.741	1.00 16.38	A
	ATOM	1572	N	ILE A		36.022	25.939		1.00 16.99	A
	ATOM	1573	CA	ILE A		35.221	25.004	19.104	1.00 16.66	A
-	ATOM	1574	CB			36.038	23.741	18.778		. A
05	ATOM	1575		ILE A		35.155	22.694	18.102	1.00 16.34	
25	MOTA	1576	CG1	ILE A		37.222	24.129	17.882	1.00 15.59 1.00 14.88	A
	ATOM	1577	CD1	ILE A		38.239	23.018	17.690		A
	ATOM	1578	С	ILE A		33.920	24.626	19.809	1.00 16.74	A
	MOTA	1579	0	ILE A		32.865	24.576	19.179	1.00 17.12	A
20	MOTA	1580	N	ILE A		33.990	24.357	21.111	1.00 16.13	A A
30	ATOM	1581	CA	ILE A		32.785	24.021	21.862	1.00 18.30	
	MOTA	1582	CB	ILE A		33.097	23.747	23.346	1.00 17.77	A
	ATOM	1583		ILE A		31.796	23.666	24.152	1.00 17.96	A
	MOTA	1584	CG1			33.877	22.437	23.481	1.00 19.55	A
25	ATOM	1585	CD1			34.446	22.217	24.886	1.00 18.64	A
35	ATOM	1586	С	ILE A		31.824	25.207	21.776	1.00 19.51	A
	ATOM	1587	0	ILE A		30.624	25.037	21.554	1.00 20.44	A
	ATOM	1588	N	TYR A		32.362	26.409	21.947	1.00 18.52	A
	ATOM	1589	CA	TYR A		31.553	27.615	21.881	1.00 20.48	A
40	MOTA	1590	СВ	TYR A		32.418	28.847	22.162	1.00 18.98	A
40	MOTA	1591	CG ·	TYR A		31.663	30.161	22.125	1.00 20.26	A
	ATOM	1592	CD1	TYR A		31.229	30.709	20.916	1.00 20.67 1.00 20.98	A A
	ATOM	1593	CE1			30.536	31.917	20.880		A A
	ATOM	1594	CD2			31.383	30.857	23.302	1.00 19.82	
4.5	ATOM	1595	CE2	TYR A		30.691	32.062	23.280	1.00 20.62	A
45	ATOM	1596	CZ	TYR A		30.271	32.587	22.067	1.00 21.15	A
	ATOM	1597	OH	TYR A		29.588	33.776	22.049	1.00 21.86	A
	ATOM	1598	С	TYR A		30.902	27.730	20.507	1.00 21.54	A
	MOTA	1599	0	TYR A		29.719	28.049	20.401	1.00 22.80	A
	ATOM	1600	N	GLN A		31.676	27.454	19.461	1.00 21.05	A
50	ATOM	1601	CA	GLN A		31.176	27.538	18.095	1.00 21.48	A
	ATOM	1602	CB	GLN A		32.323	27.341	17.097	1.00 21.41	A
	ATOM	1603	CG	GLN A		31.934	27.596	15.645	1.00 23.15	A
	ATOM	1604	CD	GLN A		33.131	27.588	14.706	1.00 24.80	A
<i>a</i> -	ATOM	1605		GLN A		34.276	27.446	15.139	1.00 22.51	A
55	MOTA	1606	NE2			32.870	27.750	13.413	1.00 22.96	A
	ATOM	1607	C ·	GLN A		30.076	26.517	17.828	1.00 21.51	A
	ATOM	1608	0	GLN A		29.123	26.806	17.108	1.00 20.50	A
	MOTA	1609	N	LEU A		30.207	25.324	18.403	1.00 21.44	A
	ATOM	1610	CA	LEU A	275	29.196	24.282	18.208	1.00 20.95	A
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	ATOM	1611	СВ	LEU .	A 275	29.645	22.958	18.846	1.00 19.11	A
	ATOM	1612	CG		A 275		22.182	18.159	1.00 21.43	A
	ATOM	1613	CD1	LEU			20.936	18.963	1.00 17.64	A
	ATOM	1614		LEU 2			21.795	16.754	1.00 20.34	A
5	ATOM	1615	C		A 275		24.697	18.815	1.00 21.32	A
•	ATOM	1616	ŏ		A 275		24.461	18.229	1.00 19.75	A
	ATOM	1617	N		A 276		25.322	19.987	1.00 19.10	A
	ATOM	1618	CA		A. 276		25.750	20.702	1.00 22.47	A
	ATOM	1619	CB		A 276		25.882	22.217	1.00 20.87	A
10	ATOM	1620		VAL			26.291	22.957	1.00 19.68	A
10	ATOM	1621	CG2		1 276 1 276		24.558	22.766	1.00 19.43	A
	ATOM	1622	C		A 276		27.075	20.211	1.00 23.89	A
	ATOM	1623	Ö		A 276		27.199	20.070	1.00 24.90	A
	ATOM	1624	N		A 277		28.062	19.965	1.00 24.56	A
15	ATOM	1625	CA		A 277		29.374	19.518	1.00 24.72	A
13	ATOM	1626	CB		A 277		30.444	19.999	1.00 24.36	A
	ATOM	1627	C		A 277		29.458	18.005	1.00 25.76	A
•	ATOM	1628	Ö		A 277		30.242	17.502	1.00 26.39	A
	ATOM	1629	N		A 278		28.651	17.280	1.00 25.13	A
20	ATOM	1630	CA		3 270 3 278		28.673	15.834	1.00 25.13	A
20	ATOM	1631	C		A 278		29.524	15.231	1.00 25.50	A
	ATOM	1632	0		278 A 278		29.510	14.015	1.00 28.17	A
	ATOM	1633	N		A 279		30.262	16.086	1.00 24.44	A
	ATOM	1634	CA		A 279		31.130	15.656	1.00 24.44	A
25	ATOM	1635	CB		A 279		32.575	15.500	1.00 25.78	A
23	ATOM	1636	CG		1 279 1 279		32.899	14.490	1.00 28.17	A
		1637		LEU A			34.344	14.684	1.00 26.17	A
	MOTA	1638	CD2				32.670	13.071	1.00 26.52	A
	MOTA	1639	CDZ		A 279		31.116	16.687	1.00 23.47	A
30	MOTA				A 279		30.994	17.882	1.00 23.47	A
30	MOTA	1640	0		1 2/9		31.239	16.236	1.00 23.35	A
	ATOM	1641	N		A 280		31.404	14.855	1.00 23.33	A
	ATOM	1642	CD				31.239	17.189	1.00 22.20	A
	ATOM	1643	CA		4 280 4 280		31.233	16.282	1.00 23.81	A
25	MOTA	1644	CB				32.020	15.073	1.00 23.24	A
35	ATOM	1645	CG		280				1.00 24.89	A
	ATOM	1646	C		1 280		32.444	18.137 17.788	1.00 22.09	A
	ATOM	1647	0		1 280		33.457 32.344		1.00 22.11	A
	ATOM	1648	N		281		31.223	19.345 19.734	1.00 23.06	A
40	ATOM	1649	CD	PRO I				20.395	1.00 21.37	A
40	ATOM	1650	CA		A 281		33.375			
	ATOM	1651	CB		281		32.751	21.509	1.00 24.89 1.00 25.24	· A
	ATOM	1652	CG		1 281		31.287	21.219		
	ATOM	1653	C		1 281		34.752	20.017	1.00 23.75	A
45	ATOM	1654	0		281	33.869	35.781	20.317	1.00 21.02	A
45	ATOM	1655	N		282		34.763	19.379	1.00 22.17	·A
	ATOM	1656	CA		282		36.007	18.998	1.00 23.16	A
	ATOM	1657	CB		282		35,943	19.406	1.00 21.01	A
	MOTA	1658	CG		282		35.482	20.822	1.00 22.66	A
~ 0	MOTA	1659		PHE 2			36.361	21.888	1.00 20.06	A
50	MOTA	1660		PHE A			34.151	21.093	1.00 20.72	A
	ATOM	1661		PHE A			35.921	23.206	1.00 22.66	A
	ATOM	1662		PHE A			33.702	22.405	1.00 20.97	A
	ATOM	1663	CZ		282		34.590	23.466	1.00 19.58	A
~~	ATOM	1664	С	PHE A		36.169	36.263	17.503	1.00 24.39	A
55	ATOM	1665	0	PHE A			35.585	16.694	1.00 25.80	A
	MOTA	1666	N	ARG A		35.355	37.248	17.142	1.00 24.99	A
	ATOM	1667	CA	ARG A			37.594	15.741	1.00 26.33	A
	MOTA	1668	CB	ARG A			37.209	15.316	1.00 28.91	A
	ATOM	1669	CG	ARG A	283	33.293	35.808	15.724	1.00 30.27	A

	ATOM	1670	CD	ARG A	A 2	28:3	31.904	35.493	15.188	1.00 33.36	A
	MOTA	1671	NE	ARG A	A 2	283 [·]	30.890	36.392	15.733	1.00 32.76	. А
	MOTA	1672	CZ	ARG A	1 2	283	30.372	36.287	16.952	1.00 34.79	A
	MOTA	1673	NH1	ARG Z	A 2	283	30.767	35.317	17.768	1.00 35.77	Α
5	MOTA	1674	NH2	ARG A	1 2	283	29.458	37.156	17.359	1.00 36.12	A
	ATOM	1675	С	ARG Z	A 2	283	35:328	39.096	15.544	1.00 26.47	A
	ATOM	1676	0	ARG A	A 2	283	35.029	39.888	16.438	1.00 26.28	A
	ATOM	1677	N	ALA A			35.818	39.486	14.373	1.00 26.70	A
	ATOM	1678	CA	ALA A			36.033	40.899	14.079	1.00 27.84	A
10	ATOM	1679	CB	ALA Z			37.188	41.442	14.914	1.00 26.24	А
10	ATOM	1680	C	ALA A			36.327	41.077	12.602	1.00 28.35	A
	ATOM	1681	Ö	ALA A			36.560	40.101	11.891	1.00 29.91	A
	ATOM	1682	N	GLY Z			36.332	42.329	12.153	1.00 29.29	A
	ATOM	1683	CA	GLY Z			36.577	42.631	10.753	1.00 29.52	A
15	ATOM	1684	C	GLY A			37.893	42.156	10.168	1.00 30.12	A
13	ATOM	1685	Ö	GLY A			37.974	41.862	8.976	1.00 30.60	A
	ATOM	1686	N	ASN A			38.939	42.097	10.983	1.00 28.49	A
	ATOM	1687	CA	ASN A			40.231	41.644	10.489	1.00 26.71	· A
		1688	CB	ASN A			41.050	42.825	9.945	1.00 26.11	A
20	ATOM		CG	ASN A			41.310	43.900	10.990	1.00 27.83	A
20	ATOM	1689 1690		ASN A			41.877	43.631	12.049	1.00 27.84	A
	MOTA			ASN A			40.908	45.131	10.685	1.00 25.95	A
	ATOM	1691		ASN A			40.997	40.924	11.584	1.00 26.03	A
	ATOM	1692	C	ASN A			40.540	40.851	12.723	1.00 25.66	A
25	ATOM	1693	0 .	GLU A			42.162	40.391	11.239	1.00 24.81	A
25	MOTA	1694	N					39.662	12.206	1.00 27.59	A
,	ATOM	1695	CA	GLU Z			42.965 44.145	38.985	11.510	1.00 27.33	A
	MOTA	1696	CB	GLU I				37.632	10.931	1.00 38.21	A
	ATOM	1697	CG	GLU Z			43.776	36.998	10.140	1.00 30.21	A
	MOTA	1698	CD	GLU Z			44.900	37.036	10.140	1.00 41.00	A
30	ATOM	1699		GLU Z			46.061 44.612	36.449	9.052	1.00 45.22	A
	MOTA	1700		GLU Z					13.383	1.00 45.22	A
	MOTA	1701	C	GLU Z			43.459	40.485	14.521	1.00 25.05	A
	MOTA	1702	0	GLU Z			43.382	41.685	13.122	1.00 23.04	A
	ATOM	1703	N	TYR			43.966	42.528	14.205	1.00 23.34	A
35	MOTA	1704	CA	TYR I			44.460		13.691	1.00 22.34	· A
	ATOM	1705	CB	TYR .			44.867	43.913	14.805	1.00 21.07	A
	ATOM	1706	CG	TYR			45.275 46.533	44.858 44.762	15.405	1.00 21.23	A
	ATOM	1707		TYR					16.475	1.00 20.43	A
40	ATOM	1708	CE1				46.891 44.380	45.588 45.809	15.302	1.00 20.43	A
40	ATOM	1709		TYR .					16.373	1.00 22.32	A
	ATOM	1710		TYR			44.725 45.981	46.637 46.518	16.953	1.00 23.20	A
	ATOM	1711	CZ	TYR .			46.316	47.313	18.024	1.00 23.18	A
	ATOM	1712	ОН	TYR .				47.513	15.288	1.00 23.10	A
	ATOM	1713	С	TYR .			43.402			1.00 22.09	A
45	ATOM	1714	0	TYR .			43.710	42.616	16.473	1.00 22.03	A
	MOTA	1715	N	LEU			42.159	42.939	14.874		Ā
	ATOM	1716	CA	LEU			41.055	43.130	15.811	1.00 21.98 1.00 22.90	A
	ATOM	1717	CB	LEU .			39.821	43.673	15.078		A
	ATOM	1718	CG	LEU .			39.896	45.130	14.601	1.00 26.52	A
50	ATOM	1719		LEU .			38.706	45.436	13.696	1.00 26.55	A
	ATOM	1720		LEU .			39.914	46.071	15.807	1.00 23.13	
	ATOM	1721	C	LEU .			40.686	41.849	16.560	1.00 21.24	A A
	ATOM	1722	0	LEU .			40.256	41.897	17.715	1.00 20.72	A
	MOTA	1723	N	ILE .			40.843	40.708	15.900	1.00 19.62	A.
55	ATOM	1724	CA	ILE .			40.538	39.433	16.533	1.00 18.54	A
	ATOM	1725	CB	ILE .			40.560	38.281	15.509	1.00 18.52	A
	ATOM	1726		ILE .			40.503	36.934	16.234	1.00 17.63	A
	ATOM	1727		ILE .			39.378	38.429	14.545	1.00 18.88	. A
	ATOM	1728	CD1	ILE .	A 2	290	39.421	37.483	13.357	1.00 19.81	A

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	ATOM	1729	С		A 290	•	41.578	39.167	17.618	1.00 19.09	A
	MOTA	1730	0	ILE A	1 290		41.236	38.788	18.737	1.00 18.20	Α
	ATOM	1731	N	PHE I	A 291	•	42.849	39.376	17.286	1.00 18.76	A
	MOTA	1732	CA		291		43.925		18.247	1.00 20.75	A
5	ATOM	1733	СВ	PHE 2			45.286	39.434	17.606	1.00 20.71	· A
,											
	ATOM	1734	CG		1 291		45.644	38.480	16.503	1.00 22.92	A
	ATOM	1735		PHE A			45.065	37.214	16.443	1.00 22.98	A
	ATOM	1736		PHE A			46.588	38.830	15.543	1.00 22.91	A
	ATOM	1737	CE1	PHE A	1 291		45.423	36.310	15.440	1.00 24.51	A
10	ATOM	1738	CE2	PHE A	291		46.954	37.931	14.535	1.00 25.54	A
	ATOM	1739	CZ	PHE A	291		46.370	36.670	14.485	1.00 23.29	Α
	ATOM	1740	С	PHE A			43.739	40.061	19.451	1.00 21.72	A
	ATOM	1741	Ō	PHE A			43.992	39.671	20.593	1.00 22.32	· A
	ATOM	1742	N	GLN A			43.284	41.275	19.178	1:00 23.27	A
15								42.264	20.216		
15	MOTA	1743	CA	GLN A			43.055			1.00 24.01	A
	MOTA	1744	CB	GLN A			42.574	43.559	19.562	1.00 25.77	A
	MOTA	1745	CG	GLN A			42.577	44.773	20.447	1.00 28.45	A
	MOTA	1746	CD	GLN A	292		42.469	46.057	19.638	1.00 29.83	A
	ATOM	1747	OE1	GLN A	292		41.520	46.244	18.872	1.00 27.16	A
20	ATOM	1748	NE2	GLN A	292		43.449	46.944	19.799	1.00 27.61	Α
	ATOM	1749	С	GLN A	292		42.018	41.733	21.204	1.00 22.97	A
	ATOM	1750	ō	GLN A			42.200	41.832	22.415	1.00 21.64	A
	ATOM	1751	N	LYS A			40.937	41.154	20.687	1.00 21.82	A
				LYS A					21.558	1.00 22.18	A
05	ATOM	1752	CA				39.895	40.612			
25	MOTA	1753	CB	LYS A			38.664	40.223	20.740	1.00 22.69	A
	ATOM	1754	CG	LYS A			37.919	41.407	20.153	1.00 25.78	Α
	ATOM	1755	CD	LYS A			36.651	40.961	19.429	1.00 27.88	A
	ATOM	1756	CE	LYS A	. 293		35.857	42.161	18.926	1.00 30.85	A
	MOTA	1757	NZ	LYS A	293		34.612	41.750	18.214	1.00 32.98	A
30	ATOM	1758	С	LYS A	293		40.398	39.398	22.343	1.00 21.20	A
	ATOM	1759	0	LYS A	293		40.041	39.204	23.509	1.00 22.01	A
	ATOM	1760	N	ILE A			41.226	38.583	21.702	1.00 19.91	A
	ATOM	1761	CA	ILE A			41.774	37.394	22.347	1.00 20.28	A
		1762	CB	ILE A			42.631	36.575	21.349	1.00 20.20	A
25	ATOM								22.098	1.00 13.30	A
35	ATOM	1763	CG2	ILE A			43.481	35.550			
	MOTA	1764		ILE A			41.716	35.897	20.318	1.00 17.93	A
	MOTA	1765		ILE A			42.467	35.237	19.178	1.00 16.21	A
	ATOM	1766	С	ILE A			42.618	37.727	23.587	1.00 21.94	· A
	ATOM	1767	0	ILE A	294		42.366	37.199	24.673	1.00 20.86	A
40	ATOM	1768	N	ILE A	295		43.610	38.600	23.439	1.00 21.88	A
	ATOM	1769	CA.	ILE A	295		44.461	38.934	24.582	1.00 24.25	Α
	ATOM	1770	CB	ILE A	295		45.668	39.805	24.175	1.00 23.93	Α
	ATOM	1771		ILE A			46.514	39.066	23.140	1.00 24.61	А
	ATOM	1772		ILE A			45.189	41.151	23.637	1.00 24.58	A
45	ATOM			ILE A				42.149			A
-45										1.00 24.80	
	ATOM	1774	C	ILE A			43.720	39.636	25.717		A
	MOTA	1775	0	ILE A		•	44.214	39.687	26.842	1.00 24.76	A
	MOTA	1776	N	LYS A			42.539	40.173	25.425	1.00 25.33	A
	MOTA	1777	CA	LYS A			41.743	40.853	26.444	1.00 26.80	A
50	ATOM	1778	CB	LYS A	296		41.178	42.170	25.894	1.00 27.39	A
	ATOM	1779	CG	LYS F	296		42.240	43.141	25.413	1.00 31.79	A
	ATOM	1780	CD	LYS A		-	41.634	44.410	24.826	1.00 35.56	А
	ATOM	1781	CE	LYS F			41.009	45.283	25.900	1.00 39.29	A
	ATOM	1782	NZ	LYS F			40.564	46.603	25.357	1.00 41.72	A
55		1783		LYS F			40.593	39.958	26.893	1.00 41.72	A
JJ	ATOM		C								
	ATOM	1784	0	LYS A			39.770	40.361	27.713	1.00 24.02	A
	ATOM	1785	N	LEU F			40.550	38.742	26.349	1.00 25.67	A
	ATOM	1786	CA	LEU F			39.500	37.777	26.666	1.00 25.16	A
	ATOM	1787	CB	LEU A	297		39.632	37.285	28.111	1.00 24.80	A

	ATOM	1788	CG	LEU A	.297	38.766	36.068	28.460	1.00 26.43	А
	MOTA	1789	CD:	l LEU A	297	39.238	34.852	27.646	1.00 26.70	A
	ATOM	1790	CD	2 LEU A	297	38.856	35.777	29.951	1.00 24.84	A
	ATOM	1791	С	LEU A	297	. 38.151	38.459	26.467	1.00 25.11	A
5	MOTA	1792	0	LEU A	297	37.261		27.309	1.00 25.28	A
	ATOM	1793	N	GLU À		38.007		25.331	1.00 24.98	A
	ATOM	1794	CA	GLU A		36.786		25.023	1.00 25.31	A
	ATOM	1795	CB	GLU A		37.143		24.291	1.00 27.13	A
	ATOM	1796	CG	GLU A		35.991	42.092	24.108	1.00 31.28	A
10	ATOM	1797	CD	GLU A		36.419		23.410	1.00 31.28	A
	ATOM	1798		L GLU A		37.348	44.027	23.918	1.00 34.40	
	ATOM	1799	OE			35.832	43.693	22.359	1.00 35.90	A
	ATOM	1800	C	GLU A		35.766		24.207		A
	ATOM	1801	o	GLU A				24.207	1.00 23.79	A
15	ATOM	1802	N			35.832	39.017		1.00 24.35	A
13				TYR A		34.825	38.427	24.902	1.00 23.45	A
	MOTA	1803	CA	TYR A		33.760	37.663	24.265	1.00 23.98	
	ATOM	1804	CB	TYR A		34.264	36.304	23.755	1.00 20.13	A
	ATOM	1805	CG	TYR A		34.348	35.233	24.828	1.00 21.17	A
20	ATOM	1806	CD1			35.336	35.279	25.810	1.00 19.32	A
20	ATOM	1807	CE1			35.389	34.332	26.826	1.00 19.30	A
	ATOM	1808		YYR A		33.410	34.201	24.888	1.00 18.96	A
	ATOM	1809		2 TYR A		33.456	33.243	25.907	1.00 19.41	A
	ATOM	1810	CZ	TYR A		34.449	33.321	26.870	1.00 18.79	A
	MOTA	1811	OH	TYR A		34.511	32.401	27.881	1.00 18.77	A
25	MOTA	1812	C	TYR A		32.699	.37.437	25.331	1.00 25.20	Α
	MOTA	1813	0	TYR A		32.942	37.681	26.506	1.00 26.46	A
	MOTA	1814	N	ASP A		31.522	36.981	24.927	1.00 26.94	A
	MOTA	1815	CA	ASP A		30.467	36.710	25.891	1.00 30.60	A
	ATOM	1816	CB	ASP A		29.665	37.981	26.179	1.00 35.86	Α
30	ATOM	1817	CG	ASP A	300	29.228	38.687	24.923	1.00 42.04	A
	ATOM	1818	OD1	ASP A	300	28.450	38.088	24.149	1.00 45.98	A
	ATOM	1819	OD2	ASP A	300	29.666	39.840	24.707	1.00 45.69	A
	MOTA	1820	С	ASP A	300	29.564	35.608	25.363	1.00 29.26	A
	ATOM	1821	0	ASP A	300	29.590	35.299	24.172	1.00 28.64	A
35	ATOM	1822	N	PHE A	301	28.778	35.011	26.253	1.00 28.96	A
	ATOM	1823	CA	PHE A	301	27.884	33.924	25.871	1.00 30.48	Α
	ATOM	1824	CB	PHE A	301	27.818	32.854	26.968	1.00 29.17	A
	ATOM	1825	CG	PHE A	301	29.147	32.279	27.356	1.00 29.29	Α
	ATOM	1826	CD1	PHE A	301	29.978	32.949	28.245	1.00 27.31	A
40	ATOM	1827	CD2	PHE A	301	29.560	31.050	26,845	1.00 27.89	. A
•	ATOM	1828	CE1	PHE A	301	31.205	32.403	28.625	1.00 28.83	A
	ATOM	1829	CE2	PHE A	301	30.781	30.498	27.217	1.00 28.05	A
	ATOM	1830	CZ	PHE A	301	31.605	31.175	28.110	1.00 28.27	A
	ATOM	1831	С	PHE A	301	26.459	34.384	25.619	1.00 32.20	A
45	ATOM	1832	0	PHE A		25.946	35.261	26.317	1.00 32.36	A
	ATOM	1833	N	PRO A		25.798	33.804	24.607	1.00 33.29	A
	ATOM	1834	CD	PRO A		26.313	32.943	23.529	1.00 34.04	A
	ATOM	1835	CA	PRO A		24.415	34.199	24.341	1.00 35.24	A
	MOTA	1836	СВ	PRO A		24.144	33.608	22.959	1.00 34.01	A
50	ATOM	1837	CG	PRO A		25.041	32.413	22.921	1.00 35.48	A
	ATOM	1838	C ·	PRO A		23.567	33.561	25.444	1.00 37.39	A
	ATOM	1839	ō	PRO A		23.935	32.518	25.986	1.00 37.33	· A
	ATOM	1840	N	ALA A		22.447	34.188	25.783	1.00 30.49	A
	ATOM	1841	CA	ALA A		21.572	33.692	26.843	1.00 39.36	A
55	ATOM	1842	CB	ALA A		20.280	34.506	26.862	1.00 40.65	A
	ATOM	1843	C	ALA A		21.238	32.197	26.814	1.00 41.88	A
	ATOM	1844	0	ALA A		21.253	31.537	27.854	1.00 41.25	
	ATOM	1845	N	ALA A						A
	ATOM	1846	CA	ALA A		20.945 20.569	31.665 30.258	25.631 25.480	1.00 41.04 1.00 40.66	A
	WI OU	TOAD	UM.	unu H	JU4	∠∪.509	JU.ZJ8	2J.48U	40.00	A

	ATOM	1847	СВ	ALA	A	304		20.121	30.004	24.040	1.00 41.36	Α
	ATOM	1848	C			304		21.628	29.223	25.876	1.00 39.61	A
	ATOM	1849	ō			304		21.298	28.156	26.395	1.00 40.61	A
	ATOM	1850	N			305		22.891	29.543	25.617	1.00 36.21	A
5	ATOM	1851	CA			305		24.022	28.662	25.909	1.00 32.08	A
•	ATOM	1852	CB			305		25.259	29.519	26.187	1.00 29.46	A
	ATOM	1853	CG			305		26.536	28.917	25.690	1.00 28.15	A
	ATOM	1854		PHE				27.146	27.875	26.377	1.00 26.20	A
	ATOM	1855	CD2			305		27.140	29.386	24.521	1.00 20.20	A
10	ATOM	1856	CE1			305		28.330	27.308	25.908	1.00 27.03	
10		1857	CE2			305		28.312	28.826			A
	ATOM					305		28.914		24.042	1.00 26.62	A
	ATOM	1858	CZ						27.786	24.737	1.00 26.61	A
	MOTA	1859	С			305 305		23.811	27.664	27.057	1.00 30.09	A
15	ATOM	1860	0					23.518	28.051	28.187	1.00 31.51	A
15	MOTA	1861	N			306		23.964	26.378	26.758	1.00 27.01	A
	ATOM	1862	CA			306		23.801	25.334	27.769	1.00 26.30	A
	ATOM	1863	CB			306		24.157	23.970	27.170	1.00 25.03	A
	MOTA	1864	CG			306		23.548	23.725	25.815	1.00 27.24	A
	MOTA	1865		PHE				22.170	23.831	25.622	1.00 28.40	Α
20	MOTA	1866		PHE				24.350	23.386	24.728	1.00 27.84	A
	MOTA	1867	CE1			306		21.601	23.603	24.365	1.00 28.05	A
	MOTA	1868	CE2					23.792	23.155	23.465	1.00 28.31	A
	ATOM`	1869	cz			306		22.415	23.263	23.283	1.00 28.00	A
	ATOM	1870	С			306		24.711	25.652	28.961	1.00 26.23	A
25	MOTA	1871	0			306		25.927	25.775	28.811	1.00 25.59	A
	MOTA	1872	N	PRO	Α	307		24.125	25.796	30.163	1.00 26.67	A
	ATOM	1873	CD	PRO	Α	307		22.685	25.625	30.430	1.00 27.95	A
	MOTA	1874	CA	PRO	Α	307		24.842	26.110	31.405	1.00 26.59	A
	ATOM	1875	CB	PRO	Α	307		23.795	25.832	32.481	1.00 26.14	A
30	ATOM	1876	CG	PRO	Α	307		22.531	26.250	31.803	1.00 27.86	A
	MOTA	1877	С	PRO	Α	307		26.145	25.355	31.659	1.00 25.58	Α
	ATOM	1878	0	PRO	Α	307		27.189	25.964	31.900	1.00 22.65	A
	ATOM	1879	N	LYS	Α	308	,	26.085	24.031	31.620	1.00 24.46	A
	ATOM	1880	CA	LYS	Α	308		27.274	23.232	31.867	1.00 23.91	A
35	ATOM	1881	CB	LYS	Α	308		26.887	21.760	32.024	1.00 23.25	. A
	ATOM	1882	CG	LYS	Α	308		26.062	21.532	33.285	1.00 28.49	A
	ATOM	1883	CD	LYS	Α	308		25.618	20.093	33.466	1.00 30.17	A
	MOTA	1884	CE	LYS	Α	308		24.760	19.973	34.722	1.00 33.12	A
	ATOM	1885	NZ	LYS	Α	308		24.122	18.636	34.860	1.00 34.13	Α
40	ATOM	1886	С	LYS	Α	308		28.314	23.426	30.769	1.00 22.84	A
	ATOM	1887	0	LYS	Α	308		29.514	23.411	31.042	1.00 22.46	A
	MOTA	1888	N	ALA	Α	309		27.861	23.621	29.534	1.00 21.59	A
	MOTA	1889	CA	ALA	Α	309		28.792	23.848	28.432	1.00 20.02	A
	ATOM	1890	CB	ALA	Α	309		28.056	23.856	27.106	1.00 18.80	A
45	ATOM	1891	Ċ	ALA	Α	309		29.481	25.191	28.662	1.00 21.41	A
	ATOM	1892	0	ALA	Α	309		30.680	25.335	28.427	1.00 21.39	A
	ATOM	1893	N	ARG	А	310		28.717	26.179	29.121	1.00 21.39	A
	ATOM	1894	CA	ARG				29,290	27.494	29.388	1.00 22.02	A
	ATOM	1895	СВ	ARG	Α	310		28.213	28.479	29.854	1.00 22.39	A
50	ATOM	1896	CG	ARG	Α	310		28.806	29.756	30.436	1.00 25.30	А
	MOTA	1897	CD	ARG				27.780	30.852	30.664	1.00 28.33	Α
	ATOM	1898	NE	ARG				28.420	32.039	31.230	1.00 30.18	A
	ATOM	1899	CZ	ARG				27.901	33.263	31.203	1.00 32.07	A
	ATOM	1900		ARG				26.719	33.477	30.634	1.00 31.19	A
55	ATOM	1901		ARG				28.567	34.277	31.742	1.00 30.49	A
	ATOM	1902	C	ARG				30.376	27.388	30.458	1.00 21.65	. A
	ATOM	1903	ŏ	ARG				31.464	27.949	30.311	1.00 20.36	A
	ATOM	1904	N	ASP				30.074	26.677	31.541	1.00 19.57	A
	ATOM	1905	CA	ASP				31.043	26.512	32.615	1.00 20.18	A
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	MOTA	1906	CB	ASP .	A 311	30.460	25.649	33.739	1.00.20.39	A
	ATOM	1907	CG	ASP	A 311	31.439	25.446	34.881	1.00 23.35	Α
	ATOM	1908		ASP		32.158	24.428	34.885	1.00 24.91	
							~			A
	MOTA	1909	OD2	ASP .		31.500	26.312	35.776	1.00 26.96	Α
5	ATOM	1910	С	ASP .	A 311	32.322	25.877	32.073	1.00 19.73	. A
	ATOM	1911	0	ASP	A 311	33.422	26.289	32.439	1.00 19.30	А
	ATOM	1912	N		A· 312	32.179	24.891	31.188	1.00 16.32	
										A
	MOTA	1913	CA		A 312	33.349	24.226	30.611	1.00 16.66	Α
	ATOM	1914	CB	LEU 2	A 312	32.927	23.035	29.744	1.00 16.12	Α
10	ATOM	1915	CG	LEU 2	4 312	34.050	22.320	28.974	1.00 14.73	A
	ATOM	1916		LEU		35.192	21.935	29.912		
									1.00 14.56	A
	ATOM	1917	CD2	LEU A		33.477	21.084	28.289	1.00 14.22	A
	ATOM	1918	C	LEU A	A 312	34.181	25.189	29.774	1.00 16.61	A
	ATOM	1919·	0	LEU Z	A 312	35.402	25.241	29.910	1.00 16.20	A
15	ATOM	1920	N	VAL 2		33.515	25.949	28.908		
13									1.00 16.20	A
	MOTA	1921	CA	VAL		34.207	26.907	28.058	1.00 15.37	A
	MOTA	1922	CB	VAL	A 313	33.216	27.648	27.130	1.00 16.42	A
	MOTA	1923	CG1	VAL A	A 313	33.915	28.796	26.426	1.00 16.93	A
	ATOM	1924		VAL 2		32.644	26.672	26.103	1.00 17.88	A
20										
20	ATOM	1925	С	VAL Z		34.960	27.923	28.911	1.00 17.39	A
	MOTA	1926	0	VAL A	A 313	36.093	28.294	28.591	1.00 18.00	A
	ATOM	1927	N	GLU Z	314	34.342	28.364	30.004	1.00 17.61	Α
	ATOM	1928	CA	GLU Z		34.986	29.331	30.885	1.00 20.43	· A
	MOTA	1929	СВ	GLU 1		34.009	29.816	31.959	1.00 22.14	A
25	MOTA	1930	CG	GLU A	314	32.800	30.550	31.396	1.00 26.52	A
	ATOM	1931	CD	GLU A	314	31.852	31.025	32.478	1.00 31.26	A
	ATOM	1932	OE1	GLU Z		31.580	30.246	33.417	1.00 33.48	А
		1933		GLU Z		31.370		32.387	1.00 34.81	A
	ATOM						32.173			
	MOTA	1934	C	GLU A		36.217	28.721	31.539	1.00 19.15	A
30	ATOM	1935	0	GLU A	314	37.134	29.433	31.934	1.00 21.47	A
	ATOM	1936	N	LYS A	315	36.245	27.400	31.651	1.00 19.51	Ą
	ATOM	1937	CA	LYS A		37.394	26.749	32.258	1.00 19.17	A
	MOTA	1938	CB	LYS A		36.946	25.514	33.043	1.00 18.84	A
	MOTA	1939	CG	LYS A	1 315	36.280	25.885	34.368	1.00 19.62	. А
35	MOTA	1940	CD	LYS A	A 315	35.653	24.696	35.073	1.00 19.22	A
	MOTA	1941	CE	LYS A		35.070	25.095	36.427	1.00 21.00	A
				LYS A		36.119	25.552	37.381	1.00 19.53	A
•	ATOM	1942	ΝZ							
	ATOM	1943	С	LYS A		38.452	26.393	31.218	1.00 18.96	A
	ATOM	1944	0 .	LYS A	315	39.511	25.873	31.561	1.00 19.85	A
40	ATOM	1945	N	LEU A	316	38.164	26.691	29.950	1.00 17.08	Α
	ATOM	1946	CA	LEU A		39.102	26.429	28.854	1.00 16.41	А
	ATOM	1947	CB	LEU A		38.414	25.636	27.738	1.00 13.81	A
	MOTA	1948	CG	LEU A	316	38.028	24.201	28.115	1.00 14.39	A
	MOTA	1949	CD1	LEU A	316	37.139	23.597	27.031	1.00 12.38	Α
45	MOTA	1950	CD2	LEU A	316	39.302	23.373	28.309	1.00 12.77	A
			С	LEU A		39.652	27.743	28.290	1.00 17.12	A
	ATOM	1951								
	MOTA	1952	0	LEU A		40.851	27.860	28.023	1.00 16.53	A
	ATOM	1953	N	LEU F	317	38.780	28.729	28.105	1.00 16.27	Α
	ATOM	1954	CA	LEU F	317	39.228	30.022	27.596	1.00 17.52	A
50	ATOM	1955	CB	LEU F		38.083	30.752	26.887	1.00 16.37	A
50										
	ATOM	1956	CG	LEU A		37.448	29.973	25.727	1.00 18.81	A
	ATOM	1957		LEU F		36.415	30.851	25.018	1.00 16.47	A
	MOTA	1958	CD2	LEU A	317	38.528	29.526	24.741	1.00 17.87	A
	ATOM	1959	С	LEU F		39.745	30.841	28.774	1.00 18.27	Α
55	•		Õ	LEU A		39.078			1.00 18.58	A
55	ATOM	1960					31.753	29.273		
	MOTA	1961	N	VAL A		40.937	30.475	29.229	1.00 18.02	A
	ATOM	1962	CA	VAL A	318	41.593	31.141	30.342	1.00 18.85	A
	MOTA	1963	СВ	VAL A	318	41.846	30.153	31.500	1.00 19.91	A
	ATOM	1964		VAL A		42.590	30.848	32.634	1.00 20.01	A
	AT OLI	エンロマ	031	A 1777 L	. 510	12.000	50.040	J2.0J4	1.00 20.01	

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	ATOM	1965	CG2	VAL A	318	40.520,	29.584	31.990	1.00 19.44	A
•	ATOM	1966	С	VAL A	318	42.923	31.657	29.811	1.00 19.67	A
	ATOM	1967	0	VAL A	318	43.690	30.902	29.208	1.00 18.26	A
	ATOM	1968	N	LEU A	319	43.197	32.939	30.028	1.00 20.07	A
5	ATOM	1969	CA	LEU A	319	44.436	33.533	29.538	1.00 20.98	A
,	ATOM	1970	СВ	LEU A		44.521	35.002	29.968	1.00 21.64	A
	ATOM	1971	CG	LEU A		43.418	35.908	29.408	1.00 24.38	A
	ATOM	1972	CD1			43.606	37.332	29.935	1.00 23.28	A
	ATOM	1973		LEU A		43.453	35.887	27.875	1.00 24.33	A
10	ATOM	1974	C	LEU A		45.680	32.774	29.994	1.00 20.38	A
10	ATOM	1975	Ö	LEU A		46.568	32.496	29.192	1.00 21.34	A
		1976	N	ASP A		45.742	32.440	31.280	1.00 20.22	A
	ATOM ATOM	1977	CA	ASP A		46.879	31.707	31.833	1.00 20.90	A
		1978	CB	ASP A	_	46.842	31.760	33.365	1.00 20.76	A
• -	MOTA		CG	ASP A		48.049	31.102	34.004	1.00 21.51	A
15	ATOM	1979		ASP A		48.669	30.226	33.367	1.00 23.46	A
	ATOM	1980		ASP A		48.371	31.450	35.159	1.00 23.89	A
	MOTA	1981		ASP A		46.814	30.247	31.367	1.00 20.06	A
	MOTA	1982	С	ASP A		45.988	29.476	31.840	1.00 20.54	A
	ATOM	1983	0			47.700	29.876	30.451	1.00 20.68	A
20	MOTA	1984	N	ALA A		47.733	28.522	29.903	1.00 22.04	A
	ATOM	1985	CA	ALA A			28.411	28.881	1.00 20.75	A
	ATOM	1986	CB	ALA A		48.860	27.400	30.940	1.00 21.62	Α.
	MOTA	1987	C	ALA A		47.858	26.259	30.665	1.00 21.99	Ā
	MOTA	1988	0	ALA A		47.482	27.715	32.127	1.00 20.89	Ä
25	MOTA	1989	N	THR A		48.372	26.698	33.167	1.00 20.82	A
	MOTA	1990	CA	THR A		48.531	27.051	34.146	1.00 20.02	A
	MOTA	1991	CB	THR A		49.670		34.848	1.00 20.19	A
	ATOM	1992	OG1			49.341	28.253	33.394	1.00 20.19	A
	MOTA	1993	CG2			50.981	27.249	33.983	1.00 21.55	A
30	ATOM	1994	C	THR A		47.264	26.498	34.894	1.00 13.33	A
	ATOM	1995	0	THR A		47.235	25.673	33.661	1.00 19.33	A
	ATOM	1996	N	LYS A		46.216	27.248	34.392	1.00 13.33	A
	MOTA	1997	CA	LYS A		44.962	27.122	35.030	1.00 21.20	A
	MOTA	1998	CB	LYS A		44.580	28.460	36.084	1.00 28.45	A
35	MOTA	1999	CG	LYS A		45.562	28.933	36.799	1.00 20.43	A
	ATOM	2000	CD	LYS A		45.055	30.177	37.802	1.00 35.70	A
	MOTA	2001	CE	LYS A		46.087	30.678	38.693	1.00 37.34	Α
	ATOM	2002	NZ	LYS A		46.532	29.569 26.614	33.539	1.00 20.68	A
	ATOM	2003	С	LYS A		43.806	26.757	33.915	1.00 20.42	A
40	MOTA	2004	0	LYS A		42.649	26.737	32.392	1.00 19.97	A
	MOTA	2005	N	ARG A		44.114	25.494	31.531	1.00 17.98	A
	ATOM	2006	CA	ARG A			25.609	30.061	1.00 15.95	A
	MOTA	2007	CB	ARG A		43.461 43.534	27.050	29.603	1.00 17.34	A
	MOTA	2008	CG	ARG A			27.030	28.172	1.00 19.80	A
45	MOTA	2009	CD	ARG A		43.996	28.565	27.944	1.00 16.93	A
	ATOM	2010	NE	ARG A		44.438		27.108	1.00 19.88	A
	MOTA	2011	CZ	ARG A		45.410	28.908	26.398	1.00 13.00	A
	ATOM	2012		ARG A		46.045	27.978		1.00 14.50	A
	ATOM	2013		ARG A		45.774	30.181	27.015 31.883	1.00 18.32	A
50	MOTA	2014	С	ARG A		42.762	24.046		1.00 18.32	A
	ATOM	2015	0	ARG A		43.673	23.222	32.006	1.00 18.20	A
	MOTA	2016	N	LEU A		41.479	23.748	32.055	1.00 18.32	·A
	MOTA	2017	CA	LEU A		41.050	22.403	32.395	1.00 17.79	A
	. ATOM	2018	CB	LEU A		39.523	22.335	32.425	1.00 17.03	A
55	MOTA	2019	CG	LEU A		38.896	21.125	33.116		A
	MOTA	2020		LEU A		39.392	21.048	34.557	1.00 15.93 1.00 16.56	A
	ATOM	2021		LEU A		37.375	21.255	33.084	1.00 18.58	A
	MOTA	2022	С	LEU A		41.599	21.433	31.356		A
	ATOM	2023	0	LEU A	√325	41.347	21.586	30.157	1.00 18.28	A

													•
	MOTA	2024	N	GLY	Д	326		42.354	20.439	31.821	1.00 1		. A
	ATOM	2025	CA			326		42.931	19.462	30.915	1.00 1		A
						326			19.558	30.807	1.00 1		A
	MOTA	2026	С						18.592	30.404	1.00 1		A
_	ATOM	2.027	0	GLY				45.093					
5	MOTA	2028	N	CYS				45.016	20.708	31.161	1.00 1		A
	ATOM	2029	CA	CYS	Α	327		46.463	20.867	31.075	1.00 1		A
	ATOM	2030	CB	CYS	Α	327		46.856	22.350	31.058	1.00 2	0.22	A
	ATOM	2031	SG	CYS	Α	327		46.782	23.200	32.649	1.00 2	1.97	A
	MOTA	2032	С	CYS	A	327		47.169	20.157	32.228	1.00 2	0.22	Ά
10	ATOM	2033	0	CYS	A·	327		46.561	19.828	33.246	1.00 1	7.92	A
	ATOM	2034	N	GLU				48.463	19.933	32.053	1.00 2	0.51	Α
	ATOM	2035	CA	GLU				49.274	19.244	33.042	1.00 2	3.34	А
	ATOM	2036	СВ			328		50.710	19.139	32.507	1.00 2		A
			CG	GLU				50.754	18.367	31.175	1.00 3		
1.5	MOTA	2037							18.500	30.414	1.00 4		A
15	ATOM	2038	CD			328		52.067			1.00 4		A
	MOTA	2039		GLU				52.535	19.643	30.218			
	MOTA	2040		GLU				52.618	17.459	29.991	1.00 4		A
	MOTĄ	2041	С			328		49.234	19.876	34.435	1.00 2		A
	ATOM	2042	0			328		49.147	19.161	35.437	1.00 2		Α
20	ATOM	2043	N	GLU	Α	329		49.276	21.204	34.506	1.00 1		. A
	ATOM	2044	CA	GLU	A	329		49.248	21.875	35.801	1.00 2		A
	ATOM	2045	CB	GLU	Α	329		49.587	23.363	35.657	1.00 2	0.36	Α
	ATOM	2046	CG	${ t GLU}$	Α	329		51.014	23.651	35.190	1.00 2	4.05	Α
	ATOM	2047	CD	GLU	Α	329		51.191	23.518	33.688	1.00 2	5.93	· A
25	ATOM	2048		GLU				50.213	23.154	32.995	1.00 2	6.61	Α
25	ATOM	2049		GLU				52.311	23.781	33.198	1.00 2	7.19	· A
	ATOM	2050	C			329		47.890	21.718	36.480	1.00 1		A
		2051				329		47.775	21.879	37.694	1.00 1		A
	ATOM					330		46.863	21.415	35.691	1.00 1		A
20	ATOM	2052	N							36.229	1.00 1		A
30	ATOM	2053	CA			330		45.520	21.220		1.00 1		A
	ATOM	2054	CB			330		44.474	21.833	35.294			
	ATOM	2055	CG			330		44.460	23.365	35.311	1.00 2		A
	ATOM	. 2056	SD	MET	A	330		44.186	24.026	36.979	1.00 2		A
	MOTA	2057	CE			330		42.435	23.712	37.186	1.00 2		A
35	MOTA	2058	С	MET	A	330		45.257	19.730	36.422	1.00 1		A
	ATOM	2059	0	MET	Α	330		44.127	19.304	36.629	1.00 1		A
	ATOM	2060	N .	GLU	Α	331		46.327	18.949	36.346	1.00 1		A
	ATOM	2061	CA	GLU	Α	331		46.289	17.501	36.531	1.00 1	7.08	Α
	ATOM	2062	CB	GLU	Α	331		45.607	17.155	37.862	1.00 1	7.00	A
40	ATOM	2063	CG			331		46.070	18.027	39.038	1.00 1	7.46	A
	ATOM	2064	CD			331		47.591	18.179	39.145	1.00 2	0.16	Α
	ATOM	2065		GLU				48.034	19.073	39.896	1.00 2	1.39	A
	ATOM	2066		GLU				48.345	17.420	38.500	1.00 1		A
	ATOM	2067	C			331		45.697	16.658	35.398	1.00 1		A
45			_		_			45.107	15.602	35.636	1.00 2		A
45	ATOM	2068	0			331					1.00 1		A
	ATOM	2069	N			332	•	45.844	17.133	34.167	1.00 1		
	ATOM	2070	CA			332	•	45.420	16.353	33.015			A
	ATOM	2071	С			332		43.982	16.154	32.596	.1.00 1		A
	ATOM	2072	0			332		43.063	16.864	33.017	1.00 1		A
50	ATOM	2073	N			333		43.804	15.141	31.750	1.00 1		A
	ATOM	2074	CA	TYR	Α	333		42.510	14.806	31.182	1.00 1		A
	ATOM	2075	CB	TYR	Α	333		42.722	13.892	29.968	1.00 1		A
	ATOM	2076	CG	TYR	A	333		43.153	14.683	28.752	1.00 1		A
	ATOM	2077		TYR	Α	333		42.206	15.172	27.849	1.00 1		A
55	ATOM	2078		TYR				42.573	16.002	26.794	1.00 1		A
	ATOM	2079		TYR				44.490	15.039	28.561	1.00 1		A
	ATOM	2080		TYR				44.872	15.877	27.499	1.00 1		A
		2081	CZ			333		43.902	16.353	26.626	1.00 1		A
	ATOM	2081				333		44.244	17.197	25.599	1.00 1		A
	ATOM	2002	On	TIK	4	JJ3		22.644	11.12/	20.000			••

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	MOTA	2083	С	TYR			41.		14.230	32,127	-	15.23	. A
	ATOM	2084	0	TYR			40.		14.323	31.846		16.63	A
	ATOM	2085	N	GLY	A	334	41.	907	13.650	33.244	1.00	15.50	A
	ATOM	2086	CA	GLY	A	334	40.	957	13.100	34.202	1.00	15.07	Α
5	ATOM	2087	С	GLY .	Α	334	39.	925	14.146	34.616	1.00	16.40	A
	ATOM	2088	0	GLY .	Α	334	38.	724	13.946	34.433	1.00	15.05	А
	ATOM	2089	N	PRO .			40.3	366	15.278	35.184		14.96	A
	ATOM	2090	CD	PRO .		-	41.		15.531	35.689		15.88	A
	ATOM	2091	CA	PRO			39.		16.339	35.606		15.29	A
10	ATOM	2092	CB	PRO .			40.		17.397	36.178		13.19	A
10			•									13.19	
	MOTA	2093	CG	PRO .			41.		16.569	36.758			A
	MOTA	2094	С	PRO .			38.		16.877	34.448		15.84	A
	MOTA	2095	0	PRO .			37.		17.204	34.631		14.84	A
	ATOM	2096	N	LEU .			39.		16.971	33.257		16.12	A
15	MOTA	2097	CA	LEU .	A	336	38.4		17.465	32.094		15.52	A
	ATOM	2098	CB	LEU .	Α	336	39.3	396	17.653	30.898	1.00	14.39	A
	ATOM	2099	CG	LEU .	A	336	38.	770	17.991	29.538	1.00	15.46	A
	ATOM	2100	CD1	LEU .	A	336	37.8	836	19.182	29.662	1.00	11.25	A
	ATOM	2101	CD2	LEU .	A	336	39.8	884	18.285	28.528	1.00	14.11	A
20	ATOM	2102	С	LEU .	Α	336	37.3	321	16.508	31.714	1.00	16.28	A
	ATOM	2103	0	LEU			36.		16.921	31.540		15.51	. A
	ATOM	2104	N	LYS .			37.		15.225	31.592		17.22	A
	ATOM	2105	CA	LYS			36.		14.243	31.235		17.39	A
		2106	CB	LYS .			37.2		12.900	30.921		17.68	A
25	ATOM	•		LYS .			38.		12.994	29.676		22.31	A
25	MOTA	2107	CG										
	ATOM	2108	CD	LYS .			39.2		11.892	29.592		24.60	A
	ATOM	2109	CE	LYS .			38.		10.560	29.189		24.76	A
	MOTA	2110	NZ	LYS .			39.		9.560	28.997		25.05	A
	ATOM	2111	С	LYS .			35.		14.096	32.342		17.33	Α
30	MOTA	2112	0	LYS .	A	337	34.	456	13.652	32.090		14.42	A
	MOTA	2113	N	ALA .	Α	338	35.	928	14.500	33.559	1.00	15.83	A
	ATOM	2114	CA	ALA .	A	338	34.	989	14.395	34.674	1.00	17.52	A
	ATOM	2115	CB	ALA .	Α	338	35.	749	14.167	35.980	1.00	19.68	A
	ATOM	2116	С	ALA .	Α	338	34.0	095	15.621	34.804	1.00	18.83	A
35	ATOM	2117	0	ALA .	Α	338	33.2	252	15.687	35.695	1.00	18.94.	A
-	ATOM	2118	N	HIS .			34.2	262	16.596	33.918	1.00	19.42	A
	ATOM	2119	CA	HIS .			33.4		17.796	34.004	1.00	19.28	Α
	ATOM	2120	СВ	HIS .			33.1		18.819	32.949	1.00	19.20	A
	ATOM	2121	CG	HIS			33.		20.134	33.074		20.26	A
40	ATOM	2122		HIS .			33.		21.299	33.649		18.95	A
70		2123		HIS .			31.		20.340	32.612		19.10	A
	ATOM	2123		HIS .			31.		21.576	32.896		22.19	A
	ATOM						32.		22.179	33.525		21.98	A
	ATOM	2125		HIS.								19.13	Ā
	ATOM	2126	C	HIS .			31.9		17.448	33.845			
45	ATOM	2127	0	HIS .			31.		16.576	33.061		19.52	
	ATOM	2128	N	PRO .			31.0		18.125	34.606		19.80	A
	MOTA	2129	CD	PRO .			31.4		19.119	35.640		19.08	Α
	MOTA	2130	CA	PRO .			29.		17.900	34.569		20.52	A
	ATOM	2131	CB	PRO .	Α	340	29.0	091	19.058	35.396		20.74	A
50	ATOM	2132	CG.	PRO .	Α	340	30.3	146	19.207	36.454	1.00	19.20	A
	ATOM	2133	С	PRO 2	Α	340	29.0	000	17.834	33.176	1.00	21.42	Α
	ATOM	2134	0	PRO I			28.0	049	17.088	32.955	1.00	22.48	A
	ATOM	2135	N	PHE			29.5		18.606	32.237		21.33	A
	ATOM	2136	CA	PHE			28.9		18.610	30.886		21.57	A
55	ATOM	2137	CB	PHE				739	19.624	30.017		21.64	A
55	ATOM	2138	CG	PHE			29.2		19.740	28.613		23.18	A
				PHE			27.9		20.171	28.382		22.58	A
	ATOM	2139		PHE						27.522		21.95	A
	ATOM	2140					30.0		19.431				
	MOTA	2141	CEI	PHE 2	Н	341	27.4	4 T O	20.292	27.082	1.00	23.54	A

	ATOM	. 2142	CE2	PHE A	3.4	1	29.533	19.548	26.220	1.00 21.83	A
	ATOM	2143	CZ	PHE A			28.228	19.980	25.998	1.00 23.23	. A
	ATOM	2144	C	PHE 2			29.055	17.226	30.237	1.00 21.84	A
	ATOM	2145	Ö	PHE A			28.232	16.896	29.389	1.00 20.37	A
5		2145		PHE A			. 30.034	16.422	30.640	1.00 20.51	A
3	ATOM		N	PHE I			30.221	15.085	30.077	1.00 23.01	A
	ATOM	2147	CA				31.710	14.809	29.850	1.00 23.01	A
	ATOM	2148	CB	PHE Z			32.398	15.812	28.971	1.00 18.00	A
	ATOM	2149	CG	PHE A				15.987			A
	ATOM	2150		PHE A			32.010		27.652	1.00 17.78	
10	ATOM	2151		PHE A			33.487	16.534	29.450	1.00 15.72	A
	ATOM	2152		PHE A			32.702	16.867	26.811	1.00 18.08	A
	ATOM	2153		PHE A			34.184	17.414	28.617	1.00 17.45	A
	MOTA	2154	CZ	PHE I			33.790	17.578	27.298	1.00 16.56	A
	MOTA	2155	С	PHE A			29.679	13.972	30.976	1.00 24.95	A
15	MOTA	2156	0	PHE A			30.002	12.798	30.777	1.00 23.95	A
	MOTA	2157	N	GLU Z	34	.3	28.861	14.333	31.958	1.00 27.35	A
	MOTA	2158	CA	GLU 1	A 34	3	28.325	13.349	32.897	1.00 30.28	A
	MOTA	2159	CB	GLU A	34	3	27.187	13.964	33.716	1.00 32.20	A
	MOTA	2160	CG	GLU A	34	3	26.581	12.991	34.714	1.00 39.71	A
20	MOTA	2161	CD	GLU Z			25.628	13.661	35.688	1.00 44.72	A
	MOTA	2162	OE1	GLU A	34	3	24.661	14.314	35.234	1.00 47.55	A
	ATOM	2163	OE2	GLU Z	A 34	3	25.847	13.526	36.911	1.00 46.89	A
	MOTA	2164	С	GLU Z	34	3	27.852	12.017	32.305	1.00 28.98	A
	MOTA	2165	0	GLU 2	A 34	3	28.225	10.952	32.800	1.00 31.73	A
25	ATOM	2166	N	SER Z	A 34	4	27.037	12.067	31.258	1.00 26.09	A
	ATOM	2167	CA	SER A	A 34	4	26.520	10.838	30.656	1.00 28.36	Α
	ATOM	2168	CB	SER	A 34	4	25.129	11.089	30.067	1.00 28.73	A
	ATOM	2169	OG	SER I	A 34	4	25.203	11.942	28.940	1.00 30.91	A
	ATOM	2170	С	SER 2	A 34	4	27.407	10.214	29.577	1.00 27.66	A
30	ATOM	2171	0	SER I	A 34	4	26.987	9.281	28.900	1.00.28.66	A
	ATOM	2172	N	VAL 2			28.627	10.715	29.419	1.00 26.75	A
	ATOM	2173	CA	VAL			29.534	10.183	28.402	1.00 23.44	A
	ATOM	2174	СВ	VAL			30.565	11.256	27.950	1.00 23.10	A
	ATOM	2175		VAL			31.589	10.631	26.995	1.00 22.24	A
35	ATOM	2176		VAL :			29.854	12.418	27.275	1.00 20.05	A
-	ATOM	2177	С	VAL			30.326	8.957	28.855	1.00 24.26	A
	ATOM	2178	0	VAL .			30.876	8.930	29.960	1.00 22.83	A
	ATOM	2179	N	THR			30.374	7.942	27.997	1.00 21.77	Α
	ATOM	2180	CA	THR			31.153	6.740	28.272	1.00 23.70	A
40	ATOM	2181	CB	THR .			30.391	5.455	27.857	1.00 26.53	A
	ATOM	2182		THR			29.248	5.284	28.706	1.00 29.98	А
	ATOM	2183		THR			31.289	4.231	27.990	1.00 24.28	A
	ATOM	2184	C	THR			32.383	6.945	27.385	1.00 23.43	A
	ATOM	2185	ō	THR			32.306	6.827	26.160	1.00 24.50	A
45	ATOM	2186		TRP			33.508		28.013	1.00 22.98	A
.5	ATOM	2187	CA	TRP			34.744	7.569	27.300	1.00 23.81	А
	ATOM	2188	CB	TRP			35.683	8.352	28.219	1.00 22.54	А
	ATOM	2189	CG	TRP			35.128	9.658	28.693	1.00 20.61	А
	ATOM	2190		TRP			35.257	10.927	28.040	1.00 19.11	Α
50	ATOM	2191		TRP			34.581	11.881	28.838	1.00 18.39	A
50	ATOM	2192		TRP			35.878	11.351	26.858	1.00 18.16	A
	ATOM	2193		TRP			34.397	9.883	29.828	1.00 18.35	A
		2194		TRP			34.065	11.218	29.923	1.00 19.51	A
•	ATOM	2194		TRP			34.510	13.234	28.491	1.00 16.88	
55	ATOM			TRP			35.808	12.701	26.511	1.00 17.23	
55	ATOM	2196		TRP			35.127	13.624	27.327	1.00 18.16	
	ATOM	2197 2198	CHZ	TRP			35.538	6.429	26.675	1.00 25.79	
	ATOM			TRP			36.304	6.654	25.742	1.00 24.67	
	ATOM	2199	O N	ALA .			35.360	5.215	27.183	1.00 27.10	
	ATOM	2200	14	ADA.	٠, ٢		55.500	J.21J	2	2.00 27.10	

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	ATOM .	2201	CA	ALA A	348	36.116	4.063	26.697	1.00 27.46	A
	ATOM	2202	СВ	ALA A	348	35.899	2.869	27.636	1.00 27.09	A
	ATOM	2203	С	ALA A	348	35.895	3.620	25.256	1.00 27.18	A
	MOTA	2204	0	ALA A	348	36.830	3.148	24.613	1.00 29.41	A
5	ATOM	2205	N	ASN A	349	34.682	3.769	24.735	1.00 26.55	A
_	ATOM	2206	CA	ASN A	349	34.418	3.310	23.375	1.00 27.28	A
	ATOM	2207	CB	ASN A	349	33.700	1.962	23.444	1.00 29.37	A
	ATOM	2208	CG	ASN A	349	32.299	2.088	24.013	1.00 30.92	Α
	MOTA	2209	OD1	ASN A		32.045	2.942	24.859	1.00 30.17	A
10	ATOM	2210	ND2	ASN A	349	31.386	1.237	23.553	1.00 33.52	A
	ATOM	2211	C .	ASN A	349	33.599	4.265	.22.509	1.00 26.47	A
	ATOM	2212	0	ASN A		32.669	~ 3.843	21.819	1.00 25.87	A
	ATOM	2213	N	LEU A	350	33.947	5.543	22.518	1.00 24.45	A
	ATOM	2214	CA	LEU A	350	33.203	6.510	21.721	1.00 23.14	A
15	ATOM	2215	СВ	LEU A		33.837	7.898	21.848	1.00 23.22	A
	ATOM	2216	CG	LEU A	350	33.659	8.605	23.191	1.00 21.05	A
	ATOM	2217	CD1	LEU A		34.646	⁻ 9.756	23.293	1.00 19.36	A
	ATOM	2218	CD2	LEU A	350	32.220	9.094	23.319	1.00 18.78	A
	ATOM	2219	С	LEU A	350	33.082	6.152	20.240	1.00 22.60	A
20	ATOM	2220	0	LEU A	350	32.011	6.296	19.650	1.00 21.15	A
	ATOM	2221	N	HIS A		34.165	5.689	19.627	1.00 23.13	A
	ATOM	2222	CA	HIS A	351	34.089	5.387	18.204	1.00 27.83	A
	ATOM	2223	CB	HIS A	351	35.506	5.325	17.596	1.00 29.36	A
	ATOM	2224	CG	HIS A		36.082	3.950	17.493	1.00 32.07	A
25	ATOM	2225	CD2	HIS A	351	36.611	3.128	18.431	1.00 32.39	A
	ATOM	2226	NĎ1	HIS A	351	36.197	3.285	16.291	1.00 33.02	A
	ATOM	2227	CE1	HIS A	351	36.775	2.113	16.493	1.00 33.58	. A
	ATOM	2228	NE2	HIS A	351	37.036	1.992	17,782	1.00 31.76	A
	ATOM	2229	С	HIS A	351	33.258	4.144	17.874	1.00 28.12	A
30	ATOM	2230	0	HIS A	351	33.015	3.847	16.707	1.00 29.49	A
	ATOM	2231	N	GLN A	352	32.800	3.442	18.908	1.00 29.28	A
	ATOM	2232	CA	GLN A	352	31.963	2.255	18.726	1.00 29.67	A
	ATOM	2233	CB	GLN A	352	32.366	1.145	19.694	1.00 30.56	A
	ATOM	2234	CG	GLN A	352	33.169	0.041	19.041	1.00 30.88	A
35	ATOM	2235	CD	GLN A	352	34.493	-0.186	19.729	1.00 31.21	A
	ATOM	2236	OE1	GLN A	352	34.541	-0.450	20.928	1.00 30.76	A
	ATOM	2237	NE2	GLN A	352	35.578	-0.084	18.971	1.00 32.30	A
	ATOM	2238	C	GLN A	352	30.504	2.638	18.963	1.00 30.42	A
	ATOM	2239	0	GLN A	.352	29.595	1.831	18.770	1.00 29.01	A
40	ATOM	2240	N	GLN A	353	30.290	3.875	19.397	1.00 27.64	A
	MOTA	2241	CA	GLN A	353	28.948	4.365	19.652	1.00 27.42	A
	ATOM	2242	CB	GLN A		28.977	5.401	20.775	1.00 25.77	A
	ATOM	2243	CG	GLN A	353	29.408	4.837	22.115	1.00 27.34	A
	MOTA	2244	CD	GLN A	353	29.638	5.914	23.156	1.00 27.19	A
45	ATOM	2245	OE1	GLN A	353	28.875	6.872	23.252	1.00 28.29	
	ATOM	2246	NE2	GLN A		30.687	5.753	23.951	1.00 28.79	А
	ATOM	2247	С	GLN A	353	28.375	4.989	18.385	1.00 29.00	A
	MOTA	2248	0	GLN A		29.118	5.455	17.516	1.00 29.14	A
	ATOM	2249	N	THR A		27.053	4.984	18.276	1.00 27.31	A
50	ATOM	2250	CA	THR A		26.390	5.568	17.119	1.00 27.85	A
	ATOM	2251	CB	THR A		24.991	4.941	16.904	1.00 30.69	A
	ATOM	2252		THR A		25.132	3.532	16.665	1.00 30.07	A
	ATOM	2253	CG2			24.289	5.585	15.709	1.00 29.58	A
	MOTA	2254	С	THR A		26.244	7.062	17.376	1.00 26.85	A
55	ATOM	2255	0	THR A		25.592	7.475	18.329	1.00 25.77	A
-	ATOM	2256	N	PRO A		26.867	7.898	16.533	1.00 27.22	A
	ATOM	2257	CD	PRO A		27.792	7.588	15.431	1.00 25.89	A
	MOTA	2258 '	CA	PRO A		26.763	9.346	16.734	1.00 27.23	A
	ATOM	2259	CB	PRO A	355	27.625	9.915	15.609	1.00 24.91	A

	ATOM	2260	CG	PRO A		28.643	8.838	15.385	1.00 25.54		A
	ATOM	2261	С	PRO A	355	25.322	9.837	16.641	1.00 28.07		Α
	AŢOM	2262	0	PRO A	355	24.548	9.364	15.810	1.00 27.24		Α
	ATOM	2263	N	PRO A	356	24.941	10.792		1.00 28.28		Α
5	ATOM	2264	CD	PRO A	356	25.752	11.560		1.00 28.31		A
	ATOM	2265	CA	PRO A	356	23.572	11.306		1.00 28.44		A
	ATOM	2266	CB	PRO A		23.539	12.301		1.00 28.11		A
	ATOM	2267	CG	PRO A		24.946	12.832		1.00 26.86		A
	ATOM	2268	C	PRO A		23.363	11.978	16.012	1.00 20.00		A
10	ATOM	2269	ō	PRO A		24.304	12.537	15.529	1.00 27.27		A
10	ATOM	2270	N	ALA A		22.143	11.910		1.00 27.27		
	ATOM	22.71	CA	ALA A		21.848	12.521	15.575			A
	ATOM	2272	CB	ALA A		20.507		14.287	1.00 32.81		A
	ATOM	2272	С	ALA A		21.824	12.019	13.757	1.00 31.99		A
1.5							14.035	14.448	1.00 35.05		A
15	MOTA	2274	0	ALA A		21.194	14.561	15.369	1.00 35.04		A
	ATOM	2275	N	LEU A		22.516	14.730	13.552	1.00 37.81		Α
	ATOM	2276	CA	LEU A		22.578	16.185	13.597	1.00 42.15		Α
	ATOM	2277	CB	LEU A		23.679	16.681	12.658	1.00 39.54		A
	ATOM	2278	CG	LEU A		25.086	16.285	13.109	1.00 39.51		Α
20	MOTA	2279		LEU A		26.102	16.686	12.062	1.00 39.29		A
	MOTA	2280		LEU A		25.395	16.953	14.445	1.00 40.01		A
	ATOM	2281	С	LEU A		21.241	16.837	13.242	1.00 45.91		A
	ATOM	2282	0	LEU A		20.874	16.927	12,069	1.00 45.71		Α
	MOTA	2283	N	THR A	359	20.530	17.290	14.275	1.00 50.06		Α
25	MOTA	2284	CA	THR A	359	19.223	17.939	14.140	1.00 53.73		Α
	MOTA	2285	CB	THR A	359	19.353	19.428	13.726	1.00 54.04	•	Α
	ATOM	2286	OG1	THR A	359	19.995	19.521	12.448	1.00 56.35		Α
	MOTA	2287	CG2	THR A	359	20.158	20.204	14.763	1.00 54.32		Α
	ATOM	2288	С	THR A	359	18.309	17.236	13.139	1.00 54.47		Α
30	ATOM	2289	0	THR A	359	18.483	16.016	12.930	1.00 55.90		Α
	ATOM	2290	OXT	THR A	359	17.407	17.908	12.595	1.00 56.97		Α
	TER										
	ATOM	1	CB	PRO B	71	99.838	54.646	-7.659	1.00 20.00	6	
	MOTA	2	CG	PRO B	71	99.216	55.105	-6.341	1.00 20.00	6	
35	ATOM	3	С	PRO B	71	98.903	54.776	-9.981	1.00 20.00	6	
	ATOM	4	0	PRO B	71	98.022		-10.109	1.00 20.00	8	
	ATOM	5	N	PRO B	71	97.782	55.851	-8.042	1.00 20.00	7	
	ATOM	6	CD	PRO B	.71	97.728	55.323	-6.668	1.00 20.00	6	
	ATOM	7	CA	PRO B	71	99.087	55.515	-8.658	1.00 20.00	6	
40	ATOM	8	N	PRO B	72	99.732		~10.985	1.00 20.00	7	
	ATOM	9	CD	PRO B	72	100.794		-10.977	1.00 20.00	6	
	ATOM	10	CA	PRO B	72	99.645		-12.297	1.00 20.00	6	
	ATOM	11	СВ	PRO B	72	100.885		-13.017	1.00 20.00	6	
	ATOM	12	CG	PRO B	72	101.026		-12.456	1.00 20.00	6	
45	ATOM	13	C	PRO B	72	99.627		-12.202	1.00 20.00	6	
	ATOM	14	Ö	PRO B	72	100.246		-11.314	1.00 20.00	8	
	ATOM	15	N	ALA B	73	98.906		-13.122	1.00 20.00	7	
	ATOM	16	CA.	ALA B	73	98.805		-13.122	1.00 20.00		
	ATOM	17	CB	ALA B	73	97.420		-12.710	1.00 20.00	6	
50	ATOM	18	C	ALA B	73	99.053				6	
50	ATOM	19	0	ALA B	73 73	99.027		-14.604 -15.526	1.00 20.00	6	
	ATOM	20	N						1.00 20.00	8	
				PRO B	74 74	99.313		-14.818	1.00 20.00	7	
	ATOM	21	CD	PRO B	74	99.473		-13.857	1.00 20.00	6	
55	ATOM	22	CA	PRO B	74	99.553		-16.189	1.00 20.00	6	
55	ATOM	23	CB	PRO B	74	99.700		-16.023	1.00 20.00	6	
	ATOM	24	CG	PRO B	74	100.292	47.004		1.00 20.00	6	
	ATOM	25	С	PRO B	74	98.371	49.018		1.00 20.00	6	
	ATOM	26	0	PRO B	74	97.279	49.296		1.00 20.00	8	
	ATOM	27	N	ALA B	75	98.589	49.037	-18.389	1.00 20.00	7	

						•						
	ATOM	28	CA	ALA.	в	75	97.516	49.368	-19.321	1.00	20.00	6
	ATOM	29	CB	ALA	в	75	98.061	49.462	-20.745	1.00	20.00	6
	ATOM	30	С	ALA	В	75	96.446	48.285	-19.246	1.00	20.00	6
	ATOM	31	0	ALA	в	75	96.745	47.126	-18.961	1.00	20.00	8
5	ATOM	32	N	LYS	в	76	95.200	48.666	-19.494	1.00	20.00	7
	ATOM	33	CA	LYS	В	76	94.098	47.716	-19.463.	1.00	20.00	6
	ATOM	34	CB	LYS	В	76	92.793	48.431	-19.805	1.00	20.00	6
	ATOM	35	CG	LYS	в	76	91.546	47.792	-19.225	1.00	20.00	6
	ATOM	36	CD	LYS	В	76	91.511		-17.711	1.00	20.00	6
10	ATOM	37	CE	LYS	в	76 ·	90.184	47.454	-17.152	1.00	20.00	6
	ATOM	38	NZ	LYS	В	76	90.108	47.606	-15.673	1.00	20.00	7
	ATOM	39	С	LYS	в 7	76 .	94.389	46.645	-20.513	1.00	20.00	б
	ATOM	40	0	LYS	в	76	94.736	46.968	-21.645	1.00	20.00	8
	ATOM	41	N	LYS	В	77	94.269	45.374	-20.145	1.00	20.00	7
15	ATOM	42	CA	LYS	в	77	94.525	44.311	-21.107	1.00	20.00	6
	MOTA	43	CB	LYS	В	77	94.875	43.008	-20.384	1.00	20.00	6
	ATOM	44	CG	LYS	В	77	96.117	43.125	-19.506	1.00	20.00	6
	ATOM	45	CD	LYS	В 7	77 .	96.461	41.812	-18.842	1.00	20.00	6
	ATOM	46	CE	LYS	В	77	97.501	42.008	-17.745	1.00	20.00	6
20	ATOM	47	NZ	LYS	В 7	77	98.771	42.582	-18.255	1.00	20.00	7
	ATOM	48	С	LYS	В	77 .	93.311	44.111	-22.012	1.00	20.00	6
	ATOM	49	0	LYS	В	77	92.218		-21.704	1.00	20.00	8
	ATOM	50	N	ARG		78	93.514		-23.129		20.00	7
	MOTA	51	CA	ARG	В	78	92.442		-24.086		20.00	6
25	MOTA	52	CB	ARG		78	92.465		-25.193		20.00	6
	MOTA	53	CG	ARG		78	93.787		-25.925		20.00	6
	ATOM	54	CD	ARG		78	93.833		-26.771		20.00	6
	ATOM	55	NE	ARG		78	95.052		-27.575		20.00	7
	MOTA	56	CZ	ARG		78 .	96.287		-27.078		20.00	6
30	ATOM	57		ARG		78	96.486		-25.764		20.00	7
	ATOM	58		ARG		78	97.330		-27.897		20.00	7
	ATOM	59	С	ARG		78	92.570		-24.678		20.00	6
	ATOM	60	0	ARG		78	93.625		-24.581		20.00	8
	ATOM	61	N	PRO	-	79	91.494		-25.303		20.00	7
35	ATOM	62	CD	PRO		79			-25.543		20.00	6
	ATOM	63	CA	PRO		79	91.519		-25.896		20.00	6 6
	ATOM	64	CB	PRO		79 70	90.214		-26.691		20.00	6
	ATOM	65	CG	PRO		79	89.304 92.737		-25.889		20.00	6
40	ATOM		. C	PRO	_	79 70	93.311		-26.778 -26.717		20.00	8
40	ATOM	67	0	PRO		79 30	93.124		-27.589		20.00	7
	ATOM	68 69	N · CA	GLU GLU		30	94.254		-28.503		20.00	6
	ATOM ATOM	70	CB	GLU		30	94.358		-29.446		20.00	6
	ATOM	71	CG	GLU		30			-28.800		20.00	6
45		72	CD	GLU		30	95.009		-29.788		20.00	6
43	ATOM ATOM	73		GLU		30	93.968		-30.308		20.00	8
	ATOM	74		GLU		30	96.150		-30.047		20.00	8
	ATOM	75	C	GLU		30	95.591		-27.787		20.00	6.
	ATOM	76	ŏ	GLU		30	96.558		-28.405		20.00	8
50	ATOM	77	N	ASP		31	95.656		-26.497		20.00	7
50	ATOM	78	CA	ASP		31	96.902		-25.749		20.00	6
	ATOM	79	CB	ASP		31	96.888		-24.446		20.00	6
	ATOM	80	CG	ASP		31	96.774		-24.682		20.00	6
	ATOM	81		ASP		31	97.436		-25.606		20.00	8
55	ATOM	82		ASP		31	96.033		-23.933		20.00	8
	ATOM	83	C	ASP		31	97.111		-25.393		20.00	6
	ATOM	84	Ō	ASP		31	98.172		-24.890		20.00	8
	ATOM	85	N	PHE		32	96.103		-25.679		20.00	7
	ATOM	86	CA	PHE		32	96.140		-25.340		20.00	6

	MOTA	87	СВ	PHE	·B	82			36.369 -24.302 1.00 20.00 6
	MOTA	88	CG	PHE		82		95.157	37.187 -23.050 1.00 20.00 6
	ATOM	89		PHE		82		95.880	36.724 -21.959 1.00 20.00 6
	MOTA	90		PHE		82		94.525	38.423 -22.961 1.00 20.00 6
5	MOTA	91		PHE		82		95.976	37.479 -20.793 1.00 20.00 6
	MOTA	92		PHE	В	82	-	94.615	39.188 -21.800 1.00 20.00 6
	MOTA	93	CZ	PHE		82		95.343	38.712 -20.713 1.00 20.00 6
	MOTA	94	С	PHE	В	82		95.929	35.719 -26.496 1.00 20.00 6
	MOTA	95	0	PHE	В	82		95.342	36.061 -27.524 1.00 20.00 8
10	MOTA	96	N	LYS	В	83		96.406	34.500 -26.286 1.00 20.00 7
	ATOM	97	CA	LYS	В	83		96.242	33.411 -27.228 1.00 20.00 6
	MOTA	98	CB	LYS	В	83		97.594	32.777 -27.562 1.00 20.00 6
	ATOM	99	CG	LYS	В	83		97.503	31.531 -28.425 1.00 20.00 6
	MOTA	100	CD	LYS	В	83		98.888	31.074 -28.856 1.00 20.00 6
15	MOTA	101	CE	LYS	В	83		98.826	29.808 -29.699 1.00 20.00 6
	MOTA	102	. NZ	LYS	В	83		98.287	28.654 -28.918 1.00 20.00 7
	MOTA	103	С	LYS	B	83		95.387	32.446 -26.416 1.00 20.00 6
	MOTA	104	0	LYS	В	83		95.884	31.776 -25.510 1.00 20.00 8
	MOTA	105	N	PHE	В	84		94.094	32.393 -26.710 1.00 20.00 7
20	ATOM	106	CA	PHE	В	84		93.217	31.511 -25.958 1.00 20.00 6
	MOTA	107	CB	PHE	В	84		91.758	31.928 -26.133 1.00 20.00 6
	MOTA	108	CG	PHE	В	84		91.426	33.228 -25.462 1.00 20.00 6
	ATOM	109	CD1	PHE	В	84		91.668	34.439 -26.099 1.00 20.00 6
	ATOM	110	CD2	PHE	В	84		90.907	33.243 -24.174 1.00 20.00 6
25	MOTA	111	CE1	PHE	В	84		91.400	35.644 -25.464 1.00 20.00 6
	MOTA	112	CE2	PHE	В	84		90.636	34.447 -23.528 1.00 20.00 6
	MOTA	113	CZ	PHE	В	84		90.884	35.646 -24.176 1,00 20.00 6
	ATOM	114	С	PHE	В	84		93.402	30.054 -26.335 1.00 20.00 6
	ATOM	115	0	PHE	В	84		93.734	29.734 -27.476 1.00 20.00 8
30	ATOM	116	N	GLY	В	85		93.196	29.178 -25.359 1.00 20.00 7
	ATOM	117	CA	GLY	В	85		93.349	27.758 -25.591 1.00 20.00 6
	MOTA	118	С	GLY	В	85		92.103	26.977 -25.221 1.00 20.00 6
	ATOM	119	Ο.	GLY	В	85		90.982	27.393 -25.525 1.00 20.00 8
	MOTA	120	N	LYS	В	86		92.296	25.858 -24.534 1.00 20.00 7
35	MOTA	121	CA	LYS	В	86		91.182	25.005 -24.153 1.00 20.00 6
	MOTA	122	CB	LYS	B	86		91.695	23.640 -23.687 1.00 20.00 6
	MOTA	123	CG	LYS	В	86		92.421	23.667 -22.356 1.00 20.00 6
	MOTA	124	CD	LYS		86		92.855	22.272 -21.941 1.00 20.00 6
	ATOM	125	CE	LYS	В	86		93.685	22.319 -20.668 1.00 20.00 6
40	MOTA	126	NZ	LYS		86		94.209	20.975 -20.287 1.00 20.00 7
	ATOM	127	C	LYS		86		90.267	25.576 -23.077 1.00 20.00 6
	MOTA	128	0	LYS		86		90.668	26.410 -22.260 1.00 20.00 8
	ATOM	129	N	ILE		87		89.026	25.106 -23.102 1.00 20.00 7
	ATOM	130	CA	ILE		87		88.023	25.497 -22.131 1.00 20.00 6
45	MOTA	131	CB	ILE		87		86.604	25.159 -22.647 1.00 20.00 6
	MOTA	132		ILE		87		85.582	25.261 -21.503 1.00 20.00 6
	MOTA	133		ILE		87		86.260	26.085 -23.820 1.00 20.00 6
	ATOM	134		ILE		87		84.912	25.819 -24.463 1.00 20.00 6
	ATOM	135	С	ILE		87		88.312	24.687 -20.872 1.00 20.00 6
50	ATOM	136	0	ILE		87		88.396	23.461 -20.927 1.00 20.00 8
	MOTA	137	N ·	LEU		88	٠	88.473	25.368 -19.742 1.00 20.00 7
	ATOM	138	CA	LEU		88		88.757	24.686 -18.486 1.00 20.00 6
	ATOM	139	CB	LEU		88		89.592	25.586 -17.575 1.00 20.00 6
	AŢOM	140	CG	LEU		88		90.968	25.987 -18.112 1.00 20.00 6
55	ATOM	141		LEU		88		91.611	27.006 -17.186 1.00 20.00 6
	ATOM	142		LEU		88		91.836	24.756 -18.234 1.00 20.00 6
	ATOM	143	С	LEU		88		87.471	24.298 -17.776 1.00 20.00 6
	ATOM	144	0	LEU		88		87.434	23.334 -17.014 1.00 20.00 8 25.051 -18.024 1.00 20.00 7
	MOTA	145	N	GLY	В	89		86.410	25.051 -18.024 1.00 20.00 7

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ATOM
                       GLY B
                               89 .
                                        85.148 24.749 -17.382
              146
                   CA
                                                                  1.00 20.00
     ATOM
                        GLY B
                               89
                                        84.038 25.599 -17.953
              147
                   С
                                                                 1.00 20.00
                                                                                6
                        GLY B
                                                26.657 -18.541
     ATOM
              148
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                                89
                                        84.296
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     MOTA
              149
                        GLU B
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                                                 25.133 -17.781
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     ATOM
              150
                   CA
                       GLU B
                                90
                                        81.629
                                                 25.832 -18.279
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                                                                               6
     ATOM
              151
                       GLU B
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                                                 25.070 -19.471
                   CB
                                                                  1.00 20.00
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                                                25.084 -20.706
     ATOM
              152
                   CG
                       GLU B
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                                        81.929
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     ATOM
              153
                   CD
                       GLU B
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                                        81.434
                                                 24.157 -21.802
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     ATOM
              154
                   OE1
                       GLU B
                              . 90
                                        81.539
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10
              155
                   OE2 GLU B
     ATOM
                               90
                                        80.935
                                                 24.662 -22.827
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              156 · C
                       GLU B
                                                 25.970 -17.188
     ATOM
                               90
                                        80.575
                                                                  1.00 20.00
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                       GLU B
                                        80.208 24.994 -16.543
     ATOM
              157
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                               90
                                                                  1.00 20.00
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     ATOM
              158
                   Ν
                       GLY B
                               91
                                        80.103
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     MOTA
              159
                       GLY B
                               91
                                        79.080
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                   CA
                                                                  1.00 20.00
                                                                               6
15
     MOTA
              160
                   С
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•	ATOM	206	N	LEU	В	98	91.617	28.690 -20.770	1.00 20.00	7
	ATOM	207	CA	LEU	В	98	93.039	28.821 -20.499	1.00 20.00	6
	ATOM	208	CB	LEU	В	98	93.727	27.459 ~20.618	1.00 20.00	6
5	ATOM	209	CG	LEU	В	98	95.240	27.421 -20.383	1.00 20.00	6
•	ATOM	210		LEU		98	95.565	28.019 -19.021	1.00 20.00	. 6
	ATOM	211		LEU		98	95.739	25.987 -20.463	1.00 20.00	6
	ATOM	212	C	LEU		98	93.580	29.785 -21.552	1.00 20.00	6
	ATOM	213	Ö	LEU		98	93.293	29.637 -22.738	1.00 20.00	8
10		214	N	ALA		99	94.343	30.783 -21.121	1.00 20.00	7
10	ATOM			ALA		99		31.767 -22.043	1.00 20.00	6
	ATOM	215	CA.				94.897			
	ATOM	216	СВ	ALA		99	94.087	33.055 -21.980	1.00 20.00	6
	ATOM	217	С	ALA		99	96.353	32.067 -21.723	1.00 20.00	6
	MOTA	218	0	ALA		99	96.748	32.110 -20.554	1.00 20.00	8
15	MOTA	219	N	ARG			97.152	32.270 -22.763	1.00 20.00	7
	ATOM	220	CA	ARG			98.554	32.596 -22.568	1.00 20.00	6
	ATOM	221	CB	ARG			99.442	31.657 -23.393	1.00 20.00	6
	ATOM	222	CG	ARG	В	100	100.934	31.833 -23.131	1.00 20.00	6
	MOTA	223	CD	ARG			101.770	30.835 -23.923	1.00 20.00	6
20	ATOM	224	NE	ARG	В	100	101.600	29.452 -23.469	1.00 20.00	7
	ATOM .	225	CZ	ARG	В	100	102.059	28.970 -22.314	1.00 20.00	6
	ATOM	226	NH1	ARG	В	100	102.722	29.752 -21.473	1.00 20.00	7
	ATOM	227	NH2	ARG	В	100	101.864	27.694 -22.003	1.00 20.00	7
	ATOM	228	С	ARG	В	100	98.756	34.045 -23.004	1.00 20.00	6
25	ATOM	229	0	ARG	В	100	98.454	34.408 -24.146	1.00 20.00	8
	ATOM	230	N	GLU	В	101	99.228	34.883 -22.087	1.00 20.00	7
	ATOM	231	CA	GLU			99.470	36.286 -22.408	1.00 20.00	6
	ATOM	232	СВ	GLU			99.709	37.091 -21.123	1,00 20.00	6
	ATOM	233	CG	GLU			99.986	38.571 -21.363	1.00 20.00	6
30	ATOM	234	CD	GLU			100.164	39.347 -20.075	1.00 20.00	6
50	ATOM	235		GLU			100.717	38.780 -19.114	1.00 20.00	8
	ATOM	236		GLU			99.765	40.531 -20.025	1.00 20.00	8
	ATOM	237	C	GLU			100.703	36.338 -23.317	1.00 20.00	6
	ATOM	238		GLU.			101.773	35.865 -22.944	1.00 20.00	8
35	ATOM	239	N -	LEU			100.546	36.909 -24.507	1.00 20.00	7
33	ATOM	240	CA	LEU			101.632	36.982 -25.482	1.00 20.00	6
	ATOM	241	CB	LEU			101.145	37.683 -26.753	1.00 20.00	6
	ATOM	242	CG	LEU			100.013	36.985 -27.517	1.00 20.00	6
		243		LEU			99.500	37.897 -28.623	1.00 20.00	6
40	ATOM	243		LEU			100.517	35.670 -28.089	1.00 20.00	6
40	ATOM							37.663 -25.000	1.00 20.00	6
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	ATOM	246	0	LEU			104.000			7
	ATOM	247	N	ALA			102.760	38.828 -24.382 39.587 -23.910	1.00 20.00 1.00 20.00	6
45	ATOM	248	CA	ALA			103.909		1.00 20.00	6
45	ATOM	249	СВ	ALA			103.464	41.002 -23.546		
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	ATOM	253	CA	THR			104.790	37.418 -20.893	1.00 20.00	6
50 ·	ATOM	254	CB	THR			104.059	37.799 -19.592	1.00 20.00	6
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55	ATOM	259	N	SER	В	105	104.042	35.274 -21.722	1.00 20.00	7
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	ATOM	261	СВ	SER	В	105	105.344	33.213 -22.048	1.00 20.00	6
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MOTA

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                   OE2 GLU B 107
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                                                                  1.00 20.00
                       ARG B 129
                                        78.351
                                                 38.554
                                                         -3.278
     MOTA
              469
                   CD
                                        77.048
                                                 39.209
                                                         -3.315
                                                                  1.00 20.00
              470
                       ARG B 129
30
     ATOM
                   NE
                                                                  1,00 20.00
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                       ARG B 129
                                        75.894
                                                 38.569
                                                         -3.484
              471
                   CZ
     MOTA
                                                                  1.00 20.00
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     ATOM
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                                                 39.248
                                                         -3.501
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                   NH2 ARG B 129
              473
     ATOM
              474
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                        ARG B 129 1
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                                                 39.788
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                                                                  1.00 20.00
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     MOTA
                                                         -5.379
                                                                  1.00 20.00
                                                                               8
                        ARG B 129
                                        82.315
                                                 39.885
35
     MOTA
              475
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                                                                  1.00 20.00
                                        81.316
                                                         -7.151
                                                                               7
                                                 38.917
              476
                        GLU B 130
     ATOM
                   N
                                        82.439
                                                         -7.421
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                       GLU B 130
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     ATOM
              477
                   CA
                                                         -8.692
                                                                  1.00 20.00
                        GLU B 130
                                        82.191
                                                 37.211
     MOTA
              478
                   CB
                                      83.408
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                                                                  1.00 20.00
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                        GLU B 130
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                   CG
     MOTA
                                                                  1.00 20.00
                                                                               6
     ATOM
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                        GLU B 130
                                        83.060
                                                 35.338 -10.168
                                                                  1.00 20.00
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                   OE1 GLU B 130
                                                 35.590 -11.061
                                        82.227
     ATOM
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     ATOM
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                                        83.708
                                                 38.853
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              483
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                                                         -6.940
                        GLU B 130
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                                                 38.575
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              484
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                                                         -8.428
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                        ARG B 131
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                                                 39.874
     ATOM
                   N
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                       ARG B 131 -
                                                 40.742
    . ATOM
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                                                                  1.00 20.00
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                                                 41.759
                                                         -9.777
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                       ARG B 131
     MOTA
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                                                 42.753 -10.035
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                   CG
                       ARG B 131
     MOTA
                                                                  1.00 20.00
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     ATOM
              489
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                       ARG B 131
                                        85.262
                                                 43.716 -11.167
                                                 44.673 -11.355
                                                                  1.00 20.00
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50
     ATOM
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                       ARG B 131
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                                                                               6
                   CZ
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                                                 45.623 -13.250
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                   NH1 ARG B 131
     ATOM
                                                                               7
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                   NH2 ARG B 131
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                                                 46.388 -12.426
     ATOM
              493
                                                                  1.00 20.00
                                        85.228
                                                 41.485
                                                         -7.409
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              494
                        ARG B 131
     MOTA
                   С
                                                         -7.071
                        ARG B 131
                                        86.413
                                                 41.500
                                                                  1.00 20.00
55
     ATOM
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                       ASP B 132
ASP B 132
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                                                 42.103
                                                         -6.715
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     ATOM
                                        84.594
                                                 42.848
                                                         -5.505
                                                                  1.00 20.00
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              497
                   CA
     MOTA
                                                                               6
                                                 43.575
                                                         -4.987
                                                                  1.00 20.00
              498
                   CB
                       ASP B 132
                                        83.350
     ATOM
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                                                 44.658
                                                         -5.943
                       ASP B 132
              499
                   CG
     MOTA
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	ATOM .	500	OD1	ASP	В	132.	83.612	45.010	-6.886	1.00	20.00	8
	ATOM	501	OD2	ASP	В	132	81.739	45.167	-5.747	1.00	20.00	. 8
	ATOM	502	С	ASP	В	132	85.192	41.969	-4.401	1.00	20.00	6
	ATOM	503	0	ASP	В	132	86.191	42.337	-3.783	1.00	20.00	8
5	ATOM	504	N	VAL	В	133	84.596	40.809	-4.150		20.00	7
	ATOM	505	CA	VAL	В	133	85.131	39.933	-3.116		20.00	6
	ATOM	506	СВ	VAL	-		84.226	38.698	-2.885		20.00	6
	ATOM	507		VAL		133	84.920	37.713	-1.957		20.00	6
	ATOM	508		VAL			82.893	39.135	-2.271		20.00	6
10	ATOM	509	C	VAL			86.540	39.470	-3.477		20.00	6
10						133	87.460					
-	MOTA	510	0	VAL				39.602	-2.675		20.00	8
	ATOM	511	N	MET		134	86.721	38.950	-4.688		20.00	7
	ATOM	512	CA	MET			88.040	38.474	-5.083		20.00	6
	ATOM	513	CB	MET		134	88.004	37.879	-6.492		20.00	6
15	ATOM	514	CG	MET			87.183	36.603	-6.573		20.00	6
	ATOM	515	SD	MET			87.477	35.650	-8.077		20.00	16
	ATOM	516	CE	MET		134	88.730	34.515	-7.475		20.00	6
	ATOM	517	С	MET		134	89.115	39.552	-4.994		20.00	6
	ATOM	518	0	MET	В	134	90.253	39.264	-4.626	1.00	20.00	8
20	ATOM	519	N	SER	В	135	88.758	40.790	-5.319	1.00	20.00	7
	ATOM	520	CA	SER	В	135	89.708	41.899	-5.260	1.00	20.00	6.
	MOTA	521	CB	SER	В	135	89.084	43.175	-5.836	1.00	20.00	6
	ATOM	522	OG	SER	В	135	88.742	43.009	-7.202	1.00	20.00	8
	ATOM	523	С	SER	В	135	90.165	42.184	-3.830	1.00	20.00	6
25	ATOM	524	0	SER	В	135	91.228	42.762	-3.614	1.00	20.00	8
	ATOM	525	N	ARG	В	136	89.354	41.782	-2.857	1.00	20.00	7
	ATOM	526	CA	ARG		136	89.672	42.013	-1.450	1.00	20.00	6
	ATOM	527	CB	ARG			88.384	42.156	-0.637		20.00	6
	ATOM	528	CG	ARG		136	87.509	43.336	-1.018		20.00	6
30	ATOM	529	CD	ARG			86.215	43.306	-0.211		20.00	6
50	ATOM	530	NE	ARG			86.491	43.117	1.209		20.00	7
	ATOM	531	CZ	ARG		136	85.565	42.888	2.132		20.00	6
	ATOM	532		ARG			84.285	42.821	1.786		20.00	7
	ATOM	533		ARG			85.920	42.715	3.401		20.00	7
35		534	C	ARG			90.506	40.891	-0.839		20.00	6
33	ATOM			ARG			91.091	41.054	0.231		20.00	8
	ATOM	535	0	LEU			90.556	39.752	-1.515		20.00	7
	ATOM	536	N				91.300		-1.005		20.00	6
	ATOM	537	CA	LEU		137		38.609				
40	MOTA	538	CB	LEU		137	90.665	37.307	-1.504		20.00	6
40	MOTA	539	CG	LEU			89.172	37.099	-1.213		20.00	6
	ATOM	540		LEU		137	88.748	35.728	-1.734		20.00	6
	ATOM	541		LEU		137	88.897	37.205	0.280		20.00	. 6
	ATOM	542	С	LEU			92.771	38.648	-1.402		20.00	6
	ATOM	543	0	LEU			93.103	38.871	-2.566		20.00	8
45	ATOM	544	N	ASP			93.645	38.436	-0.424		20.00	7
	MOTA	545	CA	ASP			95.086	38.422	-0.656		20.00	6
	ATOM	546	СВ	ASP			95.696	39.797	-0.352		20.00	6
	ATOM	547	CG	ASP			97.179	39.854	-0.674		20.00	6
	ATOM	548		ASP.			97.601	39.173	-1.634		20.00	8
50	MOTA	549	OD2	ASP	В	138	97.920	40.581	0.022	1.00	20.00	8
	ATOM	550	С	ASP			95.678	37.369	0.263	1.00	20.00	6 '
	ATOM	551	0	ASP	В	138	96.353	37.685	1.243		20.00	8
	MOTA	552	N	HIS			95.410	36.111	-0.065	1.00	20.00	7
	ATOM	553	CA	HIS			95.871	34.984	0.731		20.00	6
55	ATOM	554	СВ	HIS			94.769	34.610	1.737	1.00	20.00	6
	MOTA	555	CG	HIS			95.173	33.561	2.725		20.00	6
•	ATOM	556		HIS			95.543	33.657	4.025	1.00	20.00	6
	ATOM	557		HIS			95.241	32.221	2.405		20.00	7
	ATOM	558		HIS			95.635	31.537	3.466		20.00	6
		-										

	ATOM	559	NE2	HIS	В	139	95.825	32.385	4.461	1.00 20.00	7
	ATOM	560	С			139	96.176	33.828		1.00 20.00	
	ATOM	561	o			139	95.444	33.595		1.00 20.00	
	ATOM	562	N			140	97.257	33.080		1.00 20.00	
5	ATOM	563	CD	PRO		140	98.128	33.140		1.00 20.00	
,	ATOM	564	CA	PRO		140	97.635	31.959			
										1.00 20.00	
	ATOM	565	CB	PRO		140	98.913	31.433		1.00 20.00	-
	ATOM	566	CG	PRO		140	98.687	31.730		1.00 20.00	
	ATOM	567	С	PRO		140	96.614	30.846		1.00 20.00	
10	ATOM	568	0			140	96.747	30.107		1.00 20.00	
	ATOM	569	N	PHE		141	95.607	30.712	-0.211	1.00 20.00	7
	ATOM	570	CA	PHE	В	141	94.620	29.649	-0.398	100 20.00	6
	ATOM	571	CB	PHE	В	141	94.206	29.056	0.961	1.00 20.00	6
	ATOM	572	CG	PHE	В	141	95.321	28.335	1.681	1.00 20.00	6
15	ATOM	573	CD1	PHE	В	141	96.351	27.716	0.967	1.00 20.00	6
	ATOM	574	CD2	PHE	В	141	95.311	28.227	3.067	1.00 20.00	6
	ATOM	575		PHE			97.350	27.000	1.627	1.00 20.00	6
	ATOM	576		PHE			96.307	27.510	3.740	1.00 20.00	6
	ATOM	577	CZ	PHE		141	97.328	26.895	3.018	1.00 20.00	6
20	ATOM	578	C	PHE			93.371	30.063	-1.181	1.00 20.00	6
20	ATOM	579		PHE			92.335	29.398	-1.114		
			0							1.00 20.00	8
	ATOM	580	N	PHE			93.471	31.150	-1.934	1.00 20.00	7
	ATOM	581	CA	PHE			92.337	31.625	-2.721	1.00 20.00	6
	ATOM	582	CB	PHE			91.739	32.883	-2.082	1.00 20.00	6
25	MOTA	583	CG	PHE		142	91.048	32.628	-0.772	1.00 20.00	6
	ATOM	584		PHE		142	89.715	32.227	-0.740	1.00 20.00	6
	ATOM	585		PHE		142	91.741	32.747	0.429	1.00 20.00	6
	MOTA	586		PHE		142	89.080	31.944	0.472	1.00 20.00	6
	MOTA	587	CE2	PHE	В	142	91.116	32.465	1.647	1.00 20.00	6
30	ATOM	588	CZ	PHE	В	142	89.785	32.064	1.667	1.00 20.00	6
	MOTA	589	С	PHE	В	142	92.758	31.945	-4.146	1.00 20.00	6
	ATOM	590	0	PHE	В	142	93.865	32.429	-4.371	1.00 20.00	8
	ATOM	591	N	VAL	В	143	91.883	31.653	-5.106	1.00 20.00	7
	MOTA	592	CA	VAL	В	143	92.167	31.960	-6.504	1.00 20.00	6
35	ATOM	593	CB	VAL			91.009	31.513	-7.435	1.00 20.00	6
	ATOM	594		VAL		143	91.116	32.209	-8.795	1.00 20.00	6
	ATOM	595		VAL			91.061	30.000	-7.623	1.00 20.00	6
	ATOM	596	C	VAL			92.301	33.469	-6.545	1.00 20.00	6
	ATOM	597	Ö	VAL			91.505	34.179	-5.932	1.00 20.00	8
40	ATOM	598	N	LYS		144	93.312	33.957	-7.252	1.00 20.00	7
70		599		LYS		144				1.00 20.00	
	ATOM		CA				93.547	35.392	-7.340		6
	ATOM	600	CB	LYS		144	95.051	35.689	-7.267	1.00 20.00	6
	ATOM	601	CG	LYS		144	95.382	37.182	-7.318	1.00 20.00	6
	ATOM	602	CD	LYS			96.881	37.441	-7.201	1.00 20.00	6
45	ATOM	603	CE	LYS			97.191	38.936	-7.298	1.00 20.00	6
	MOTA	604	NZ	LYS			98.661	39.215	-7.246	1.00 20.00	7
	ATOM	605	С	LYS			92.989	36.003	-8.614	1.00 20.00	6
	ATOM	606	0	LYS			92.993	35.371	-9.675	1.00 20.00	8
	ATOM	607	N	LEU	В	145	92.495	37.230	-8.490	1.00 20.00	7
50	ATOM	608	CA	LEU	В	145	91.968	37.975	-9.624	1.00 20.00	6
	ATOM	609	CB	LEU	В	145	90.678	38.703	-9.234	1.00 20.00	6
	MOTA	610	CG	LEU			89.938		-10.326	1.00 20.00	6
	ATOM	611		LEU			88.611	39.992	-9.782	1.00 20.00	6
	ATOM	612		LEU			90.791		-10.806	1.00 20.00	6
55	ATOM	613	C	LEU			93.059	38.984	-9.968	1.00 20.00	6
-	ATOM	614	0	LEU			93.291	39.940	-9.216	1.00 20.00	8
	ATOM	615	N	TYR			93.735		-11.093	1.00 20.00	7
	ATOM	616	CA	TYR						1.00 20.00	6
							94.815		-11.517		
	ATOM	617 ⁻	CB	TYR	D	740	95.821	30.904	-12.389	1.00 20.00	6

	ATOM	618	CG	TYR :	В.	146	96.624	37.858 -11.661 1.00 20.00 6
	ATOM	619	CD1	TYR I	В	146	96.139	36.559 -11.498 1.00 20.00 6
	ATOM	620	CE1	TYR I	В	146	96.894	35.589 -10.836 1.00 20.00 6
	ATOM	621	CD2	TYR	В	146	97.878	38.165 -11.140 1.00 20.00 6
5	ATOM	622	CE2	TYR I		_	98.639	37.208 -10.476 1.00 20.00 6
	ATOM	623	CZ	TYR			98.144	35.925 -10.331 1.00 20.00 6
	ATOM	624	ОН	TYR			98.920	34.981 -9.706 1.00 20.00 8
	ATOM	625	C	TYR			94.357	40.884 -12.293 1.00 20.00 6
	ATOM	626	Ö	TYR			94.933	41.963 -12.160 1.00 20.00 8
10	ATOM	627	N	PHE			93.326	40.722 -13.110 1.00 20.00 7
10	ATOM	628	CA	PHE 1			92.855	41.832 -13.923 1.00 20.00 6
	ATOM	629	CB	PHE			93.823	42.044 -15.092 1.00 20.00 6
	ATOM	630	CG	PHE			94.027	40.809 -15.945 1.00 20.00 6
		631		PHE I			93.049	40.397 -16.850 1.00 20.00 6
15	ATOM						95.188	40.047 -15.822 1.00 20.00 6
15	MOTA	632		PHE I				
	MOTA	633		PHE I			93.221	
	ATOM	634		PHE I			95.372	
	ATOM	635	CZ	PHE			94.388	38.490 -17.485 1.00 20.00 6
00	ATOM	636	C	PHE I			91.473	41.566 -14.480 1.00 20.00 6
20	ATOM	637	0	PHE !			90.972	40.442 -14.423 1.00 20.00 8
	ATOM	638	N	THR I			90.865	42.616 -15.021 1.00 20.00 7
	ATOM	639	CA	THR I			89.560	42.509 -15.643 1.00 20.00 6
	MOTA	640	CB	THR			88.402	42.889 -14.678 1.00 20.00 6
	ATOM	641	OG1	THR I			88.492	44.275 -14.338 1.00 20.00 8
25	ATOM	642		THR			88.460	42.057 -13.403 1.00 20.00 6
	ATOM	643	С	THR			89.532	43.469 -16.821 1.00 20.00 6
	ATOM	644	0	THR			90.281	44.448 -16.866 1.00 20.00 8
	ATOM	645	N	PHE I			88.685	43.161 -17.791 1.00 20.00 7
	ATOM	646	CA	PHE I			88.508	44.011 -18.948 1.00 20.00 6
30	ATOM	647	CB	PHE I			89.750	44.013 -19.864 1.00 20.00 6
	ATOM	648	CG	PHE I			90.133	42.664 -20.419 1.00 20.00 6 42.182 -21.587 1.00 20.00 6
	MOTA	649		PHE I			89.552	_
		650		PHE I			91.122	
0.5	ATOM	651		PHE I			89.953	
35	ATOM	652		PHE I			91.532	40.681 -20.345 1.00 20.00 6
	ATOM	653	CZ	PHE I			90.948	40.213 -21.517 1.00 20.00 6
	ATOM	654	С	PHE			87.271	43.498 -19.649 1.00 20.00 6
	ATOM	655	0	PHE I			86.714	42.474 -19.251 1.00.20.00 8
4.0	ATOM	656	N	GLN			86.812	44.221 -20.657 1.00 20.00 7
40	ATOM	657	CA	GLN I			85.619	43.807 -21.372 1.00 20.00 6
	ATOM	658	CB	GLN I			84.358	44.260 -20.614 1.00 20.00 6
	ATOM	659	CG	GLN I			84.302	45.761 -20.289 1.00 20.00 6
	ATOM	660	CD	GLN I			83.011	46.172 -19.567 1.00 20.00 6
4.5	ATOM	661		GLN I			81.970	46.385 -20.196 1.00 20.00 8 46.273 -18.240 1.00 20.00 7
45	MOTA	662		GLN I			83.078	2012.0
	ATOM	663	С	GLN I			85.598	44.400 -22.760 1.00 20.00 6
	ATOM	664	0	GLN I			86.281	45.387 -23.033 1.00 20.00 8
	ATOM	665	N	ASP I			84.846	43.766 -23.649 1.00 20.00 7
	MOTA	666	CA	ASP I			84.683	44.296 -24.992 1.00 20.00 6
50	ATOM	667	CB	ASP I			85.160	43.312 -26.074 1.00 20.00 6
	ATOM	668	CG	ASP 1			84.558	41.934 -25.939 1.00 20.00 6
	ATOM	669		ASP I			83.425	41.812 -25.436 1.00 20.00 8
	ATOM	670		ASP I			85.227	40.963 -26.365 1.00 20.00 8
	MOTA	671	С	ASP 1			83.188	44.573 -25.095 1.00 20.00 6
55	ATOM	672	0	ASP I			82.501	44.610 -24.069 1.00 20.00 8
	MOTA	673	N	ASP 1			82.669	44.758 -26.301 1.00 20.00 7
	ATOM	674	CA	ASP 1			81.251	45.062 -26.437 1.00 20.00 6
	MOTA	675	CB	ASP I			80.907	45.346 -27.901 1.00 20.00 6
	ATOM	676	CG	ASP I	В	152	81.616	46.574 -28.432 1.00 20.00 6

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677
                   OD1 ASP B 152
                                       81.748
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                                                                  1.00 20.00
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                   OD2 ASP B 152
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                                                 46.563 -29.613
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     ATOM
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                       ASP B 152
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                                                 44.020 -25.888
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	ATOM	798	CG	LEU			89.408	18.363	-2.569	1.00 20.00	6
5	ATOM	799		LEU			90.769	17.703	-2.412	1.00 20.00	6
•	ATOM	800		LEU			89.065	19.193	-1.338	1.00 20.00	6
	ATOM	801	C	LEU			88.757	17.394	-5.346	1.00 20.00	6
	ATOM	802	Ö	LEU			89.124	16.283	-4.968	1.00 20.00	8
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10	ATOM	804	CA	LEU			86.647	16.500	-6.153	1.00 20.00	6
10	ATOM	805	CB	LEU			85.364	17.014	-6.809	1.00 20.00	6
	ATOM	806	CG	LEU			84.292	15.977	-7.168	1.00 20.00	6
	ATOM	807		LEU			83.883	15.186	-5.929	1.00 20.00	6
	ATOM	808		LEU			83.083	16.687	-7.756	1.00 20.00	6
15	ATOM	809	C	LEU			87.290	15.440	-7.046	1.00 20.00	6
15	ATOM	810	Ö	LEU			87.091	14.243	-6.845	1.00 20.00	8
		811	N	LYS			88.068	15.888	-8.027	1.00 20.00	7
	ATOM ATOM	812	CA	LYS			88.727	14.967	-8.941	1.00 20.00	6
		813	CB			169	89.610	15.729	-9.930	1.00 20.00	6
20	ATOM	814	CG	LYS			90.379		-10.882	1.00 20.00	6
20	ATOM	815	CD	LYS			91.226		-11.877	1.00 20.00	6
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	ATOM	817	NZ	LYS			93.253		-12.173	1.00 20.00	7
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	ATOM	822					93.217	15.010	-6.624	1.00 20.00	6
20	ATOM	823	CG			170	94.347	14.331	-7.085	1.00 20.00	6
30	ATOM	824		TYR				14.900	-8.036	1.00 20.00	6
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35	ATOM	829	OH			170		12.622	-5.499	1.00 20.00	6
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40	ATOM	834	CB			171	87.278		-2.791	1.00 20.00	6
	ATOM	835		ILE			86.367	12.065	-2.603	1.00 20.00	6
	ATOM	836		ILE			87.764	14.141 14.990	-2.019	1.00 20.00	6
	ATOM	837		ILE			86.652 87.994	11.066	-4.931	1.00 20.00	6
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45	ATOM		0				88.030	9.925 11.331	-6.156	1.00 20.00	7
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50	ATOM	843	CG			172	85.094	11.658	-9.259	1.00 20.00	6
50	ATOM	844	CD			172	84.352	11.981	-9.063	1.00 20.00	7
	ATOM	845	NE			172	83.187	12.843		1.00 20.00	6
	ATOM	846	CZ			172	82.192	12.589	-8.217 -7.469	1.00 20.00	7
	ATOM	847		ARG			82.209	11.491	-7.469	1.00 20.00	7
 -	ATOM	848		ARG			81.168	13.428	-8.127	1.00 20.00	6
55	ATOM	849	C			172	88.202	9.378	-7.497	1.00 20.00	8
	ATOM	850	0			172	88.050	8.160	-7.587	1.00 20.00	7
	MOTA	851	N			173	89.348	9.985	-7.783		6
	ATOM	852	CA			173	90.509	9.244	-8.256 -8.603	1.00 20.00	6
	ATOM	853	CB	LYS	В	173	91.647	10.206	-8.603	1.00 20.00	O

		054			_				0 511	. 0.45	1 00 00 0	
	ATOM	854	CĢ	LYS				92.930	9.511	-9.045	1.00 20.0	
	ATOM	855	CD	LYS				94.081	10.496	-9.222	1.00 20.0	
	ATOM	856	CE	LYS	В	173		93.862		-10.406	1.00 20.0) 6
	ATOM	857	ΝZ	LYS	В	173		93.858	10.711	-11.715	1.00 20.0	7
5	ATOM	858	С	LYS	В	173		91.025	8.191	-7.280	1.00 20.0	6 (
	ATOM	859	Ö	LYS	В	173		91.274	7.055	-7.674	1.00 20.0	8 (
	ATOM	860	N	ILE	В	174		91.192	8.554	-6.012	1.00 20.0	7
	ATOM	861	CA	ILE				91.710	7.593	-5.042	1.00 20.0	
	MOTA	862	СВ	ILE				92.884	8.191		1.00 20.0	
10	ATOM	863		ILE				93.970	8.701	-5.166	1.00 20.0	
10	ATOM	864		ILE				92.394	9.337	-3.343	1.00 20.0	
	ATOM	865		ILE				93.480	9.916	-2.457	1.00 20.00	
		866							7.030	-4.074	1.00 20.00	
	MOTA		C	ILE				90.674				
1.5	ATOM	867	0	ILE				91.025	6.296	-3.151	1.00 20.00	
15	ATOM	868	N	GLY				89.405	7.367	-4.283	1.00 20.00	
	ATOM	869	CA	GLY				88.359	6.855	-3.413	1.00 20.00	
	MOTA	870	С	GLY				88.160	7.650	-2.138	1.00 20.00	
	ATOM	871	0	GLY				87.083	8.198	-1.905	1.00 20.00	
	MOTA	872	N	SER	В	176		89.192	7.701	-1.304	1.00 20.00	
20	ATOM	873	CA	SER	В	176		89.140	8.447	-0.053	1.00 20.00) 6
	ATOM	874	CB	SER	В	176		88.395	7.653	1.026	1.00 20.00) 6
	ATOM	875	OG	SER	В	176		89.150	6.543	1.472	1.00 20.00	8 (
	ATOM	876	С	SER	В	176		90.565	8.742	0.401	1.00 20.00	6
	ATOM	877	0	SER	В	176		91.506	8.049	0.009	1.00 20.00	8 (
25	ATOM	878	N	PHE	В	177		90.718	9.769	1.228	1.00 20.00	7
	ATOM	879	CA	PHE	В	177		92.029	10.184	1.722	1.00 20.00) 6
	ATOM	880	CB	PHE				92.028	11.694	1.990	1.00 20.00	
	ATOM	881	CG	PHE				92.002	12.546	0.747	1.00 20.00	
	ATOM	882		PHE				91.484	12.060	-0.449	1.00 20.00	
30	ATOM	883		PHE				92.481	13.855	0.787	1.00 20.00	
50	ATOM	884		PHE				91.443	12.860	-1.585	1.00 20.00	
	ATOM	885		PHE				92.444	14.665	-0.343	1.00 20.00	
	ATOM	886	CZ	PHE				91.925	14.168	-1.532	1.00 20.00	
								92.427		3.009	1.00 20.00	
25	ATOM	887	C	PHE					9.475			
35	ATOM	888	0	PHE				91.582	9.223	3.872	1.00 20.00	
	ATOM	889	N	ASP		178		93.711	9.152	3.147	1.00 20.00	
	MOTA	890	CA	ASP				94.155	8.529	4.385	1.00 20.00	
	ATOM	891	CB	ASP				95.581	7.972	4.267	1.00 20.00	
	ATOM	892	CG	ASP				96.594	9.018	3.845	1.00 20.00	
40	ATOM	893		ASP				96.392	10.214	4.139	1.00 20.00	
	ATOM	894		ASP		178		97.612	8.634	3.230	1.00 20.00	
	ATOM	895	С	ASP		178		94.092	9.640	5.436	1.00 20.00	
•	ATOM	896	0	ASP				93.736	10.778	5.117	1.00 20.00	
	ATOM	897	N	GLU				94.443		6.677	1.00 20.00	
45	ATOM	898	CA	GLU	В	179		94.380	10.311	7.744		
	ATOM	899	CB	GLU	В	179		94.623	9.637	9.096	1.00 20.00	6
	ATOM	900	CG	GLU	В	179		94.747	10.611	10.255	1.00 20.00	6
	ATOM	901	CD	GLU	В	179		94.331	9.994	11.574	1.00 20.00	6
	ATOM	902	OE1	GLU	В	179		94.589	8.789	11.770	1.00 20.00	
50	ATOM	903		GLU				93.753	10.717	12.416	1.00 20.00	
	ATOM	904	С	GLU				95.320	11.501	7.575	1.00 20.00	
	ATOM	905	ō	GLU				94.948	12.636	7.881	1.00 20.00	
	ATOM	906	N	THR				96.528	11.246	7.086	1.00 20.00	
	ATOM	907	CA	THR				97.509	12.308	6.886	1.00 20.00	
55	ATOM	908	CB	THR			•	98.866	11.720	6.445	1.00 20.00	
23	ATOM	909	OG1	THR				99.349	10.842	7.466	1.00 20.00	
		910						99.888		6.213	1.00 20.00	
	ATOM			THR					12.825		1.00 20.00	
	ATOM	911	C	THR				97.040	13.331	5.849		
	ATOM	912	0	THR	Þ	TAN		97.136	14.542	6.069	1.00 20.00	8

	MOTA	913	N	CYS	В	181	96.534	12.845	4.721	1.00 20.00	7
	ATOM	914	CA	CYS	В	181	96.057	13.733	3.666	1.00 20.00	6
	ATOM	915	СВ	CYS	В	181	95.836	12.945	2.375	1.00 20.00	6
	ATOM	916	SG	CYS	В	181	97.372	12.255	1.685	1.00 20.00	
5	ATOM	917	C	CYS	В	181	94.775	14.449	4.079	1.00 20.00	
_	ATOM	918	0	CYS			94.570	15.615	3.733	1.00 20.00	
	ATOM	919	N	THR			93.914	13.755	4.820	1.00 20.00	
	ATOM	920	CA	THR			92.669	14.356	5.286	1.00 20.00	
	ATOM	921	CB	THR			91.812	13.354	6.103		
10	ATOM	922	OG1							1.00 20.00	
10							91.372	12.283	5.259	1.00 20.00	
	ATOM	923	CG2				90.600	14.054	6.690	1.00 20.00	
	ATOM	924	. C	THR			93.014	15.535	6.196	1.00 20.00	
	ATOM	925	0	THR			92.515	16.649	6.019	1.00 20.00	
	MOTA	926	И.	ARG			93.873	15.273	7.175	1.00 20.00	
15	MOTA	927	CA	ARG			94.299	16.293	8.121	1.00 20.00	
	MOTA	928	CB	ARG	В	183	95.311	15.707	9.109	1.00 20.00	6
	ATOM	929	CG	ARG	В	183	95.957	16.744	10.012	1.00 20.00	6
	ATOM	930	CD	ARG	В	183	96.886	16.116	11.050	1.00 20.00	6
	ATOM	931	NE	ARG	В	183	96.167	15.220	11.949	1.00 20.00	
20	ATOM	932	CZ	ARG			96.098	13.900	11.804	1.00 20.00	
	ATOM	933		ARG			96.717	13.306	10.791	1.00 20.00	
	ATOM	934		ARG			95.389	13.176	12.664	1.00 20.00	
	ATOM	935	C-	ARG			94.923	17.505	7.427	1.00 20.00	
•	ATOM	936	Ö	ARG		_	94.545	18.646	7.698	1.00 20.00	
25	ATOM	937	N	PHE			95.877	17.264	6.534	1.00 20.00	
23	ATOM	938	CA	PHE		184	96.539	18.367	5.847		
										1.00 20.00	
	ATOM	939	CB	PHE			97.610	17.847	4.889	1.00 20.00	
	ATOM	940	CG	PHE			98.387	18.943	4.223	1.00 20.00	
20		941		PHE		184	99.451	19.555	4.879	1.00 20.00	
30	MOTA	942		PHE			98.009	19.415	2.975	1.00 20.00	6
	MOTA	943		PHE			100.125	20.627	4.301	1.00 20.00	6
	ATOM	944		PHE		184	98.676	20.491	2.388	1.00 20.00	
	ATOM	945	CZ	PHE			99.735	21.097	3.053	1.00 20.00	. 6
	ATOM	946	С	PHE			95.580	19.267	5.066	1.00 20.00	6
35	MOTA	947	0	PHE	В	184	95.567	20.481	5.255	1.00 20.00	8
	ATOM	948	N	TYR	В	185	94.784	18.679	4.181	1.00 20.00	7
	MOTA	949	CA	TYR	В	185	93.854	19.471	3.390	1.00 20.00	. 6
	ATOM	950	CB	TYR	В	185	93.305	18.634	2.236	1.00 20.00	6
	ATOM	951	CG	TYR	В	185	94.337	18.504	1.140	1.00 20.00	6
40	ATOM	952	CD1	TYR	В	185	94.611	19.580	0.293	1.00 20.00	6
	ATOM	953	CE1	TYR	В	185	95.637	19.516	-0.643	1.00 20.00	6
	ATOM	954		TYR			95.118	17.352	1.017	1.00 20.00	6
	ATOM	955	CE2				96.152	17.282	0.081	1.00 20.00	6
	ATOM	956	CZ	TYR			96.405	18.367	-0.742	1.00 20.00	6
45	ATOM	957	ОН	TYR			97.436	18.314	-1.657	1.00 20.00	8
	ATOM	958	C	TYR			92.738	20.098	4.208	1.00 20.00	6
	ATOM	959	Ö	TYR			92.286	21.195	3.891	1.00 20.00	
											8
	ATOM	960	N	THR			92.303	19.422	5.267	1.00 20.00	7
60	ATOM	961	CA	THR			91.265	19.987	6:122	1.00 20.00	6
50	ATOM	962	CB	THR			. 90.799	18.996	7.219	1.00 20.00	6
	ATOM	963		THR			90.193	17.846	6.606	1.00 20.00	8
	ATOM	964		THR			89.774	19.671	8.144	1.00 20.00	6
	ATOM	965	С	THR			91.858	21.218	6.805	1.00 20.00	6
	ATOM	966	0	THR			91.188	22.242	6.948	1.00 20.00	8
55	ATOM	967	N	ALA			93.120	21.115	7.222	1.00 20.00	7
	MOTA	968	CA	ALA			93.787	22.234	7.882	1.00 20.00	6
	ATOM	969	CB	ALA	В	187	95.184	21.817	8.349	1.00 20.00	6
	ATOM	970	С	ALA	В	187	93.879	23.449	6.946	1.00 20.00	6
	ATOM	971	0	ALA	В	187	. 93.654	24.585	7.372	1.00 20.00	8

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	ATOM	972	N	GLU	В	188		94.205	23.22	2 5.674	1.00	20.00	7
•	ATOM	973	CA	GLΰ	В	188		94.292	24.34	3 4.740	1.00	20.00	6
	ATOM	974	СВ	GLU	В	188		94.843	23.89	8 3.376	1.00	20.00	6
	ATOM	975	CG	GLU	В	188		96.285	23.39	1 3.407	1.00	20.00	6
5	ATOM	976	CD			188.		97.030	23.63		1.00	20.00	6
,	ATOM	977		GLU				96.407	23.53		1.00	20.00	8
		978		GLU				98.247	23.93		1.00		8
	ATOM			GLU				92.912	24.97		1.00		6
	MOTA	979	С	GLU				92.782	26.19		1.00		8
10	ATOM	980	0					91.875	24.15		1.00		7
10	MOTA	981	N	ILE					24.13			20.00	6
	ATOM	982	CA	ILE				90.530				20.00	6
	ATOM	983	CB	ILE				89.495	23.56		1.00		6
	ATOM	984	CG2					88.094	24.15		1.00		6
	ATOM	985	CG1	ILE				89.855	22.77				
15	MOTA	986	CD1					89.058	21.48			20.00	6
	MOTA	987	С	ILE				90.152	25.51		1.00		6
	MOTA	988	0	ILE				89.634	26.63		1.00		. 8
	MOTA	989	N	VAL				90.412	24.97		1.00		7
	ATOM	990	CA	$_{ m LAV}$				90.116	25.67			20.00	6
20	MOTA	991	CB	VAL				90.557	24.84		1.00		6
	MOTA	992		VAL				90.540	25.71		1.00		6
	MOTA	993	CG2	VAL				89.643	23.64		1.00		6
	MOTA	994	С	VAL				90.865	27.01			20.00	6
	MOTA	995	0	VAL				90.311	28.03		1.00		8
25	MOTA	996	N	SER				92.125	26.99			20.00	7
	MOTA	997	CA	SER				92.934	28.21			20.00	6
	MOTA	998	CB			191		94.378	27.88			20.00	6
	ATOM	999	OG	SER	В	191		95.220	29.00			20.00	8
	MOTA	1000	С	SER	В	191		92.361	29.24			20.00	6
30	ATOM	1001	0			191		92.351	30.44			20.00	8
	MOTA	1002	N	ALA	В	192		91.882	28.75			20.00	7
	MOTA	1003	CA	ALA	В	192		91.306	29.63			20.00	6
	MOTA	1004	CB	ALA	В	192		91.006	28.85			20.00	6
	ATOM	1005	С	ALA	В	192		90.029	30.25			20.00	6
35	ATOM	1006	0	ALA	В	192		89.799	31.45			20.00	8
	ATOM	1007	N	LEU	В			89.203	29.43			20.00	7
	ATOM	1008	CA	LEU	В	193		87.957	29.94			20.00	6
	ATOM	1009	CB	LEU	В	193	•	87.101	28.78			20.00	6
	MOTA	1010	CG	LEU	В	193		86.447	27.89			20.00	6
40	ATOM	1011	CD1	LEU	В	193		85.645	26.77			20.00	6
	MOTA	1012	CD2	LEU	В	193		85.530	28.75			20.00	6
	ATOM	1013	С	LEU	В	193		88.215	30.95			20.00	6
	ATOM	1014	0	LEU	В	193		87.474	31.93	5 7.435		20.00	8
	ATOM	1015	N	GLU	В	194		89.254	30.73			20.00	, 7
45	MOTA	1016	CA	GLU	В	194		89.562	31.69	9 9.157		20.00	6
	ATOM	1017	CB	GLU	В	194		90.773	31.25	7 9.982		20.00	6
	ATOM	1018	CG	GLU	В	194		91.288	32.35	3 10.914		20.00	6
	ATOM	1019	CD	GLU	В	194		92.381	31.87			20.00	6
	ATOM	1020	OE1	GLU	В	194		93.246	31.09	0 11.420	1.00	20.00	8
50	ATOM	1021	OE2	GLU	В	194		92.376	32.31	2 13.031	1.00	20.00	8
	ATOM	1022	С	GLU	В	194		89.847	33.05	3 8.511	1.00	20.00	6
	ATOM	1023	0	GLU	В	194		89.375	34.08	3 8.972	1.00	20.00	8
	ATOM	1024	N			195		90.608	33.04	6 7.426	1.00	20.00	7
	ATOM	1025	CA	TYR	в	195		90.928	34.29		1.00	20.00	6
55	ATOM	1026	СВ			195		91.919	34.04		1.00	20.00	6
	ATOM	1027	CG			195		92.193	35.27		1.00	20.00	6
	ATOM	1028		TYR				93.098	36.24	4 5.202	1.00	20.00	6
•	ATOM	1029	CE1			195		93.356	37.38	2 4.429	1.00	20.00	6
	ATOM	1030		TYR				91.545	35.46	1. 3.553	1.00	20.00	6
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ATOM
             1031
                    CE2 TYR B 195
                                         91.794
                                                  36.591
                                                            2.775
                                                                   1.00 20.00
     ATOM
             1032
                    CZ
                        TYR B 195
                                         92.701
                                                  37.545
                                                                   1.00 20.00
                                                            3.219
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     MOTA
             1033
                    OH
                        TYR B 195
                                         92.956
                                                  38.656
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     ATOM
             1034
                         TYR B 195
                                         89.668
                    С
                                                  34.923
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     ATOM
             1035
                        TYR B 195
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                    O
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     ATOM
             1036
                        LEU B 196
                                         88.885
                    N
                                                  34.103
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     ATOM
             1037
                        LEU B 196
                                         87.664
                    CA
                                                  34.576
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     MOTA
             1038
                        LEU B 196
                                         86.972
                    CB
                                                  33.426
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                                                                                 6
     ATOM
             1039
                                         85.933
                    CG
                        LEU B 196
                                                  33.824
                                                            3.060
                                                                   1.00 20.00
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10
     ATOM
             1040
                    CD1 LEU B 196
                                         86.602
                                                  34.659
                                                           1.966
                                                                   1.00 20.00
                                                                                6
     MOTA
             1041
                    CD2 LEU B 196
                                         85.305
                                                  32.568
                                                           2.463
                                                                   1.00 20.00
                                                                                 6
     MOTA
             1042
                                                  35.161
                    С
                        LEU B 196
                                         86.731
                                                           5.888
                                                                   1.00 20.00
     ATOM
             1043
                    0
                        LEU B 196
                                         86.299
                                                  36.308
                                                           5.774
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     ATOM
             1044
                    N
                        HIS B 197
                                         86.431
                                                  34.378
                                                           6.917
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15
     ATOM
             1045
                        HIS B 197
                                         85.533
                    CA
                                                  34.840
                                                           7.967
                                                                   1.00 20.00
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     ATOM
             1046
                        HIS B 197
                                         85.241
                    CB
                                                  33.697
                                                           8.942
                                                                   1.00 20.00
                                                                                6
     ATOM
             1047
                    CG
                        HIS B 197
                                         84.377
                                                 32.622
                                                           8.356
                                                                   1.00 20.00
                                                                                6
     ATOM
             1048
                    CD2 HIS B 197
                                         83.734
                                                 32.550
                                                           7.163
                                                                   1.00 20.00
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     ATOM
             1049
                    ND1 HIS B 197
                                         84.083
                                                 31.452
                                                           9.022
                                                                   1.00 20.00
20
     ATOM
             1050
                    CE1 HIS B 197
                                         83.296
                                                 30.704
                                                           8.264
                                                                   1.00 20.00
                                                                                б
     ATOM
             1051
                    NE2 HIS B 197
                                        83.071
                                                 31.346
                                                           7.132
                                                                   1.00 20.00
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     ATOM
                        HIS B 197
                                        86.080
                                                 36.060
             1052
                    C
                                                           8.697
                                                                   1.00 20.00
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                                       85.314
                                                 36.919
     ATOM
             1053
                    0
                        HIS B 197
                                                           9.146
                                                                   1.00 20.00
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     ATOM
             1054
                    N
                        GLY B 198
                                        87.404
                                                 36.143
                                                           8.804
                                                                   1.00 20.00
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     ATOM
             1055
                        GLY B 198
                                        88.009
                                                 37.285
                    ÇA
                                                           9.464
                                                                   1.00 20.00
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                                        87.687
     MOTA
             1056
                        GLY B 198
                                                 38.580
                    С
                                                           8.737
                                                                   1.00 20.00
                                                                                6
     ATOM
             1057
                    0
                        GLY B 198
                                        87.784
                                                 39.661
                                                           9.311
                                                                   1.00 20.00
                                                                                8
     ATOM
             1058
                        LYS B 199
                                        87.308
                                                 38.475
                    N
                                                           7.466
                                                                   1.00 20.00
                                                                                7
             1059
                        LYS B 199
     ATOM
                    CA
                                        86.959
                                                 39.652
                                                           6.674
                                                                   1.00 20.00
                                                                                6
     MOTA
             1060
                    СВ
                        LYS B 199
                                        87.577
                                                 39.573
                                                           5.279
                                                                   1.00 20.00
                                                                                6
             1061
     MOTA
                    CG
                        LYS B 199
                                        89.082
                                                 39.736
                                                           5.258
                                                                   1.00 20.00
                                                                                6
     ATOM
             1062
                    CD
                        LYS B 199
                                        89.574
                                                 39.919
                                                           3.833
                                                                   1.00 20.00
                                                                                6
     ATOM
             1063
                   CE
                        LYS B 199
                                        91.054
                                                 40.243
                                                           3.807
                                                                   1.00 20.00
                                                                                6
     ATOM
             1064
                   NZ
                        LYS B 199
                                        91.398
                                                 41.382
                                                           4.706
                                                                   1.00 20.00
                                                                                7
     MOTA
             1065
                        LYS B 199
                                                 39.804
                                                                   1.00 20.00
                   C
                                        85.451
                                                           6.539
                                                                                6
     ATOM
             1066
                        LYS B 199
                                                                  1.00 20.00
                   0
                                        84.972
                                                 40.556
                                                           5.693
                                                                                8
     MOTA
             1067
                   N
                        GLY B 200
                                        84.707
                                                 39.079
                                                           7.368
                                                                   1.00 20.00
                                                                                7
     ATOM
             1068
                        GLY B 200
                                        83.258
                   CA
                                                 39.158
                                                           7.328
                                                                   1.00 20.00
                                                                                6
     ATOM
             1069
                   С
                        GLY B 200
                                        82.646
                                                 38.660
                                                           6.032
                                                                   1.00 20.00
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40
     ATOM
             1070
                        GLY B 200
                                                                   1.00 20.00
                   0
                                        81.644
                                                 39.198
                                                           5.564
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     ATOM
             1071
                   N
                        ILE B 201
                                        83.243
                                                 37.630
                                                                   1.00 20.00
                                                           5.445
                                                                                7
     ATOM
             1072
                        ILE B 201
                                        82.726
                                                 37.075
                   CA
                                                           4.205
                                                                   1.00 20.00
                                                                                6
     ATOM
             1073
                        ILE B 201
                   CB
                                        83.775
                                                 37.140
                                                                   1.00 20.00
                                                           3.080
                                                                                6
     ATOM
             1074
                   CG2 ILE B 201
                                      83.257
                                                 36.413
                                                                   1.00 20.00
                                                           1.841
                                                                                6
45
     MOTA
             1075
                   CG1 ILE B 201
                                      84.109
                                                 38.599
                                                           2.761
                                                                   1.00 20.00
                                                                                6
                   CD1 ILE B 201
     MOTA
             1076
                                      85.330
                                                 38.758
                                                                   1.00 20.00
                                                           1.870
                                                                                6
     ATOM
             1077
                   С
                        ILE B 201
                                      82.329
                                                 35.623
                                                           4.395
                                                                   1.00 20.00
                                        83.094
     ATOM
            1078
                   0
                        ILE B 201
                                                 34.826
                                                           4.942
                                                                   1.00 20.00
                                                                                8
     ATOM
            1079
                        ILE B 202
                                                                  1.00 20.00
                   N
                                        81.125
                                                 35.291
                                                           3.940
                                                                                7
50
    ATOM
            1080
                   CA
                        ILE B 202
                                        80.592
                                                 33.936
                                                           4.016
                                                                  1.00 20.00
                                                                                6
                       ILE B 202
    ATOM
            1081
                   CB
                                        79.119
                                                 33.953
                                                           4.481
                                                                  1.00 20.00
                                                                                6
                   CG2 ILE B 202
                                                 32.522
    ATOM
            1082
                                        78.583
                                                           4.595
                                                                   1.00 20.00
                                                                                6
    ATOM
            1083
                   CG1 ILE B 202
                                        79.008
                                                 34.675
                                                           5.825
                                                                  1.00 20.00
                                                                                6
                                        77.576
                                                 34.865
     ATOM
            1084
                   CD1 ILE B 202
                                                                  1.00 20.00
                                                           6.294
                                                                                6
55
                        ILE B 202
     ATOM
            1085
                   С
                                        80.644
                                                 33.393
                                                           2.589
                                                                  1.00 20.00
                                                                                6
    ATOM
            1086
                   0
                        ILE B 202
                                       80.182
                                                 34.056
                                                           1.663
                                                                  1.00 20.00
    ATOM
            1087
                       HIS B 203
                   N
                                        81.204
                                                 32.204
                                                           2.395
                                                                  1.00 20.00
                                                                                7
    ATOM
            1088
                   CA
                       HIS B 203
                                        81.279
                                                 31.652
                                                           1.044
                                                                  1.00 20.00
                                                                                6
    ATOM
            1089
                   CB
                       HIS B 203
                                        82.258
                                                 30.480
                                                           0.999
                                                                  1.00 20.00
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	ATOM	1090	CG	HIS	В	203		82.478	29.942	-0.380	1.00 20.00) 6
	MOTA	1091	CD2	HIS	В	203	•	81.646	29.282	-1.220	1.00 20.00	
	ATOM	1092	ND1	HIS	В	203		83.659	30.116	-1.069	1.00 20.00	
	ATOM	1093	CE1	HIS	В	203		83.545	29.588	-2.275	1.00 20.00	
5	ATOM	1094	NE2	HIS	В	203		82.333	29.076	-2.392	1.00 20.00	
	ATOM	1095	С			203		79.896	31.211	0.530	1.00 20.00	
	ATOM	1096	0	HIS	В	203		79.508	31.546	-0.593	1.00 20.00	
	ATOM	1097	N	ARG				79.168	30.458	1.357	1,00 20.00	
	ATOM	1098	CA	ARG				77.819	29.969	1.039	1.00 20.00	
10	ATOM	1099	CB	ARG	В	204		76.916	31.117	0.583	1.00 20.00	
	MOTA	1100	CG	ARG	В	204		76.601	32.120	1.675	1.00 20.00	
	MOTA	1101	CD	ARG				75.316	32.878	1.377	1.00 20.00	
	MOTA	1102	NE	ARG	В	204		75.376	33.616	0.119	1.00 20.00	
	ATOM	1103	CZ	ARG	В	204		74.423	34.443	-0.303	1.00 20.00	
15	ATOM	1104	NH1	ARG	В	204		73.336	34.636	0.436	1.00 20.00	
	ATOM	1105		ARG				74.555	35.084	-1.457	1.00 20.00	
•	ATOM	1106	С	ARG				77.700	28.829	0.030	1.00 20.00	
	ATOM	1107	0	ARG				76.611	28.300	-0.177	1.00 20.00	
	ATOM	1108	N	ASP				78.792	28.456	-0.620	1.00 20.00	
20	ATOM	1109	CA	ASP				78.718	27.342	-1.550	1.00 20.00	
	ATOM	1110	СВ	ASP				78.380	27.829	-2.961	1.00 20.00	
	ATOM	1111	CG	ASP				77.941	26.694	-3.867	1.00 20.00	
	ATOM	1112	OD1	ASP	В	205		77.544	25,638	-3.330	1.00 20.00	
	ATOM	1113		ASP				77.982	26.853	-5.104	1.00 20.00	
25	ATOM	1114	С	ASP	В	205		80.019	26.560	-1.547	1.00 20.00	
	ATOM	1115	0	ASP				80.508	26.122	-2.588	1.00 20.00	
	ATOM	1116	N	LEU				80.573	26.375	-0.354	1.00 20.00	
	ATOM	1117	CA	LEU	В	206		81.819	25.652	-0.208	1.00 20.00	6
	ATOM	1118	СВ	LEU			•	82.361	25.826	1.212	1.00 20.00	
30	ATOM	1119	CG	LEU				83.764	25.271	1.471	1.00 20.00	'6
	ATOM	1120		LEU				84.765	25.969	0.561	1.00 20.00	
	ATOM .	1121		LEU		206		84.135	25.477	2.933	1.00 20.00	6
	MOTA	1122	С	LEU	В	206		81.609	24.174	-0.514	1.00 20.00	6
	ATOM	1123	Ο.	LEU	В	206		80.691	23.549	0.011	1.00 20.00	8
35	ATOM	1124	N	LYS	В	207		82.461	23.628	-1.375	1.00 20.00	7
	MOTA	1125	CA	LYS	В	207		82.379	22.223	-1.765	1.00 20.00	. 6
	MOTA	1126	СВ	LYS	В	207		81.160	22.000	-2.679	1.00 20.00	6
	ATOM	1127	CG	LYS	В	207		81.130	22.913	-3.893	1.00 20.00	6
	ATOM	1128	CD	LYS	В	207		79.876	22.720	-4.736	1.00 20.00	6
40	ATOM	1129	CE	LYS	В	207		79.788	23.797	-5.813	1.00 20.00	6
	ATOM	1130	NZ	LYS	В	207		78.695	23.557	-6.791	1.00 20.00	7
	ATOM	1131	С	LYS	В	207		83.657	21.808	-2.487	1.00 20.00	6
	ATOM	1132	0	LYS	В	207		84.416	22.656	-2.960	1.00 20.00	8
	ATOM	1133	N	PRO	В	208		83.916	20.494	-2.582	1.00 20.00	7
45	MOTA	1134	CD	PRO	В	208		83.153	19.378	-1.993	1.00 20.00	6
	MOTA	1135	CA	PRO				85.122	20.005	-3.259	1.00 20.00	
	ATOM	1136	CB	PRO				84.922	18.494	-3.267	1.00 20.00	6
	ATOM	1137	CG	PRO				84.174	18.256	-1.984	1.00 20.00	. 6
	MOTA	1138	С	PRO				85.303	20.574	-4.666	1.00 20.00	6
50	ATOM	1139	0	PRO	В	208		86.431	20.752	-5.124	1.00 20.00	8
	ATOM	1140	N	GLU				84.197	20.859	-5.347	1.00 20.00	7
	ATOM	1141	CA	GLU				84.243	21.410	-6.705	1.00 20.00	6
	ATOM	1142	CB	GLU				82.836	21.424	-7.317	1.00 20.00	6
	ATOM	1143	CG	GLU				82.755	22.081	-8.690	1.00 20.00	6
55	ATOM	1144	CD	GLU				81.323	22.296	-9.159	1.00 20.00	6
	ATOM	1145		GLU				80.587	21.299	-9.322	1.00 20.00	8
	ATOM	1146		GLU				80.933	23.465	-9.364	1.00 20.00	8
	ATOM	1147	C	GLU				84.810	22.836	-6.716	1.00 20.00	6
	ATOM	1148	ō	GLU				85.409	23.269	-7.705	1.00 20.00	- 8
	212 023		~		_			20.103				J

	MOTA	1149	N			210	84.604	23.549		1.00 20.00	
	MOTA	1150	CA	ASN	В	210	85.051	24.932		1.00 20.00	
	MOTA	1151	CB	ASN	В	210	84.033	25.695	-4.588	1.00 20.00	6
	ATOM	1152	CG	ASN	В	210	82.851	26.170	-5.396	1.00 20.00	6
5	ATOM	1153	OD1	ASN	В	210	81.807	26.520	-4.846	1.00 20.00	8
	ATOM	1154		ASN			83.010	26.194	-6.717	1.00 20.00	7
	ATOM	1155	C			210	86.427	25.070	-4.797	1.00 20.00	6
	ATOM	1156	ō			210	86.937	26.181	-4.641	1.00 20.00	
	ATOM	1157	N			211	87.016	23.948	-4.406	1.00 20.00	
10		1158	CA			211	88.331	23.958	-3.790	1.00 20.00	
10	ATOM					211		23.990	-2.521	1.00 20.00	
	ATOM	1159	CB				88.336			1.00 20.00	
	ATOM	1160		ILE			89.732	23.025	-1.925		
	ATOM	1161	CG1			211	87.350	23.682	-1.510	1.00 20.00	
	ATOM	1162		ILE			87.121	22.832	-0.285	1.00 20.00	
15	MOTA	1163	С			211	89.307	23.414	-4.816	1.00 20.00	
	MOTA	1164	0	ILE	В	211	89.475	22.199	,-4.949	1.00 20.00	
	ATOM	1165	N	LEU	В	212	89.938	24.319	-5.558	1.00 20.00	7
	ATOM	1166	CA	LEU	В	212	90.875	23.918	-6.601	1.00 20.00	6
	ATOM	1167	СВ	LEU	В	212	90.966	25.012	-7.673	1.00 20.00	6
20	ATOM	1168	CG	LEU	В	212	89.630	25.510	-8.235	1.00 20.00	6
	ATOM	1169		LEU			89.896	26.462	-9.390	1.00 20.00	6
	ATOM	1170		LEU			88.781	24.331	-8.709	1.00 20.00	
	ATOM	1171	C			212	92.254	23.628	-6.038	1.00 20.00	
	ATOM	1172	Ö			212	92.537	23.923	-4.873	1.00 20.00	8
25	ATOM	1173	N			213	93.114	23.053	-6.875	1.00 20.00	
25						213	94.472	22.714	-6.472	1.00 20.00	
	ATOM	1174	CA							1.00 20.00	
	ATOM	1175	CB			213	94.609	21.192	-6.388		
•	MOTA	1176	CG			213	93.775	20.526	-5.292	1.00 20.00	
	MOTA	1177		LEU			93.737	19.035	-5.508	1.00 20.00	
30	ATOM	1178		LEU			94.374	20.852	-3.935	1.00 20.00	6
	ATOM	1179	С			213	95.503	23.277	-7.449	1.00 20.00	6
	MOTA	1180	0	LEU	В	213	95.422	23.033	-8.657	1.00 20.00	
	MOTA	1181	N	ASN	В	214	96.470	24.036	-6.940	1.00 20.00	
	ATOM	1182	CA	ASN	В	214	97.488	24.585	-7.826	1.00 20.00	6
35	ATOM	1183	CB	ASN	В	214	98.198	25.792	-7.201	1.00 20.00	6
	ATOM	1184	CG	-		214	98.938	25.448	-5.927	1.00 20.00	6
	ATOM	1185	OD1	ASN	В	214	99.267	24.288	-5.669	1.00 20.00	8
	ATOM	1186		ASN			99.224	26.469	-5.123	1.00 20.00	7
	ATOM	1187	С			214	98.508	23.515	-8.182	1.00 20.00	6
40	ATOM	1188	Ō			214	98.420	22.372	-7.725	1.00 20.00	8
	ATOM	1189	N			215	99.482	23.894	-8.996	1.00 20.00	
	ATOM	1190	CA			215	100.514	22.965	-9.430	1.00 20.00	6
	ATOM	1191	CB	GLU			101.491		-10.362	1.00 20.00	6
	ATOM	1191					102.544	•	-10.302	1.00 20.00	6
45			CG			215					
45	ATOM	1193	CD			215	103.323		-12.080	1.00 20.00	6
	MOTA	1194		GLU			103.909		-11.810	1.00 20.00	8
•	ATOM	1195		GLU			103.344		-13.215	1.00 20.00	8
	MOTA	1196	С			215	101.275	22.307	-8.274	1.00 20.00	6
	MOTA	1197	0			215	101.801	21.205	-8.428	1.00 20.00	8
50	ATOM	1198	N			216	101.335	22.976	-7.123	1.00 20.00	7
	MOTA	1199	CA	ASP	В	216	102.036	22.430	-5.958	1.00 20.00	6
	ATOM	1200	CB	ASP	В	216	102.727	23.549	-5.179	1.00 20.00	6
	ATOM	1201	CG	ASP	В	216	103.952	24.086	5.896	1.00 20,00	6
	ATOM	1202	OD1	ASP			104.766	23.267	-6.376	1.00 20.00	8
55	ATOM	1203		ASP			104.110	25.323	-5.973	1.00 20.00	8
;	ATOM	1204	C			216	101.121	21.651	-5.013	1.00 20.00	6
	ATOM	1205	Ö			216	101.532	21.241	-3.925	1.00 20.00	8
	ATOM	1205	N	MET			99.877	21.463	-5.434	1.00 20.00	7
		1200	CA	MET			98.890	20.730	-4.657	1.00 20.00	6
	ATOM	1201	CM	Lini	J	211	20.020	20.130	± . UJ /	2.00 20.00	•

	ATOM	1208	СВ	MET			99.402	19.319	-4.358		20.00	6
	ATOM	1209	CG	MET			99.456	18.432	-5.601		20.00	6
	ATOM	1210	SD	MET			97.857	18.342	-6.445		20.00	
	ATOM	1211	CE	MET			97.073	16.984	-5.543		20.00	6
5	ATOM	1212	С	MET	В	217	98.397	21.403	-3.373		20.00	6
	MOTA	1213	Ο.	MET			97.972	20.730	-2.435		20.00	8
	ATOM	1214	N	HIS			98.469	22.730	-3.331		20.00	7
	ATOM	1215	CA	HIS			97.949	23.487	-2.197		20.00	б
	ATOM	1216	CB	HIS			98.831	24.700	-1.898		20.00	6
10	ATOM	1217	CG	HIS			100.100	24.357	-1.177		20.00	6
	ATOM	1218	CD2	HIS	В	218	101.390	24.362	-1.588		20.00	6
	ATOM	1219		HIS			100.117	23.935	0.136		20.00	7
	MOTA	1220		HIS			101.364	23.698	0.504		20.00	6
	ATOM	1221	NE2	HIS			102.156	23.947	-0.524		20.00	7
15	MOTA	1222	С	HIS			96.583	23.939	-2.703		20.00	6
	ATOM	1223	0	HIS			96.400	24.090	-3.910		20.00	.8
	ATOM	1224	N	ILE			95.628	24.160	-1.808		20.00	7
	MOTA	1225	CA	ILE			94.301	24.562	-2.257		20.00	6
	ATOM	1226	СВ	ILE			93.232	24.359	-1.159		20.00	6
20	MOTA	1227		ILE			93.266	22.918	-0.654	1.00		6
	MOTA	1228		ILE				25.353	-0.011		20.00	6
	ATOM	1229		ILE			92.351	25.342	1.036		20.00	6
	MOTA	1230	С	ILE			94.207	26.010	-2.714		20.00	6 8
	MOTA	1231	0	ILE			95.044	26.850	-2.375		20.00	7
25	ATOM	1232	N	GLN			93.168	26.274	-3.497		20.00	6
	ATOM	1233	CA	GLN			92.859	27.600	-3.999 -5.350		20.00	6
	ATOM	1234	CB			220	93.537	27.867 28.246	-5.216		20.00	6
	ATOM	1235	CG			220	95.011 95.599	28.799	-6.503		20.00	6
	MOTA	1236	CD			220	95.725	28.086	-7.502		20.00	8
30	MOTA	1237		GLN GLN			95.723	30.079	-6.486		20.00	7
	ATOM	1238				220	91.350	27.626	-4.140		20.00	6
•	ATOM	1239 1240	С 0			220	90.792	27.133	-5.124		20.00	8
	MOTA	1240	N			221	90.689	28.178	-3.129		20.00	7
35	ATOM ATOM	1241	CA			221	89.240	28.260	-3.122		20.00	6
33	ATOM	1242	CB			221	88.731	28.550	-1.700		20.00	6
	ATOM	1243		ILE			87.209	28.707	-1.708		20.00	6
	ATOM	1245	CG1			221	89.164	27.406	-0.773		20.00	6
	ATOM	1246		ILE			88.743	27.559	0.668	1.00	20.00	6
40	ATOM	1247	C			221	88.760	29.339	-4.092	1.00	20.00	6
-10	ATOM	1248	ŏ			221	89.411	30.374	-4.262	1.00	20.00	8
	ATOM	1249	N			222	87.633	29.082	-4.748	1.00	20.00	7
	ATOM	1250	CA	THR	В	222	87.084	30.039	-5.701		20.00	6
	ATOM	1251	CB	THR	В	222	87.565	29.728	-7.125		20.00	6
45	ATOM	1252	OG1	THR	В	222	87.179	30.795	-8.000	1.00	20.00	8
	ATOM	1253		THR			86.962	28.410	-7.618	1.00	20.00	6
	ATOM	1254	С			222	85.554	30.028	-5.683	1.00	20.00	6
	ATOM	1255	0	THR	В	222	84.950	29.417	-4.791	1.00	20.00	8
	ATOM	1256	N	ASP	В	223	84.949	30.712	-6.659		20.00	7
50	ATOM	1257	CA	ASP	В	223	83.492	30.806	-6.806		20.00	6
	MOTA	1258	CB			223	82.872	29.399	-6.767		20.00	6
	MOTA	1259	CG			223	81.414	29.384	-7.205		20.00	6
	ATOM	1260	OD1	ASP	В	223	80.990	30.335	-7.900		20.00	8
	ATOM	1261	OD2	ASP			80.701	28.414	-6.866		20.00	8
55	ATOM	1262	С			223	82.878	31.694	-5.725		20.00	6
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	ATOM	1264	N			224	83.105	33.001	-5.848		20.00	7
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	ATOM	1509	CB	SER	В	262	77.806	28.913	11.895	1.00 2		6
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-	ATOM	1515	CB	SER		263	76.132	28.750	6.507	1.00 2		
	ATOM	1516	OG			263	75.011		7.156	1.00 2		8
15	ATOM	1517	C	SER		263	78.123	27.244	6.737	1.00 2		6
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35	MOTA	1537	CB	TRP		266	77.167	23.384	8.148	1.00 2		6.
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	ATOM	1540	CE2	TRP		266	74.881	20.455	7.542	1.00 2		6
	ATOM	1541	CE3	TRP		266	75.117	22.010	9.785	1.00 2		6
40	MOTA	1542	CD1	TRP		266	76.220	21.792		1.00 2		6
	ATOM	1543	NE1	TRP		266	75.365	20.719	6.288	1.00 2		7
	ATOM	1544	CZ2	TRP		266	73.988	19.466	7.975	1.00 2		6
	ATOM	1545	CZ3	TRP		266	74.227	20.359	10.216	1.00 2		.6
	ATOM	1546	CH2				73.674	19.434	9.310	1.00 2		6
45	ATOM	1547	С	TRP			79.169	22.356	7.038	1.00 2		6
	ATOM	1548	0	TRP			79.356	21.142	6.988	1.00 2		8
	MOTA	1549	N	ALA			79.411	23.164		1.00 2		7
	ATOM	1550	CA	ALA			79.930	22.646	4.751	1.00 2		6
	ATOM	1551	CB	ALA			80.089	23.772	3.746	1.00 2		6
50	ATOM	1552	С	ALA	В	267	81.277	21.976	5.016	1.00 2	0.00	6
,	MOTA	1553	0	ALA			81.570	20.914	4.471	1.00 2		8
	ATOM	1554	N	LEU			82.091	22.596	5.864	1.00 2	0.00	7
	ATOM	1555	CA	LEU	В	268	83.393	22.030	6.209	1.00 2		6
	MOTA	1556	CB	LEU			84.092	22.898	7.264	1.00 2		6.
55	ATOM	1557	CG	LEU			85.379	22.332	7.879	1.00 2		6
	ATOM	1558	CD1	LEU	В	268	86.442	22.192	6.803	1.00 2	•	6
	ATOM	1559	CD2	LEU	В	268	85.872	23.263	9.006	1.00 2		6
•	ATOM	1560	C .	TE U			83.193	20.617	6.753	1.00 2		6
	ATOM	1561	0	LEU	В	268	83.903	19.684	6.372	1.00 2	0.00	8

	MOTA	1562	N	GLY	В	269		82.220	20.463	7.645	1.00	20.00	7
	ATOM	1563	CA	GLY			•	81.947	19.156	8.217		20.00	6
	ATOM	1564	С	GLY				81.597	18.125	7.156	1.00	20.00	6
	ATOM	1565	0	GLY				82.025	16.971	7.239	1.00	20.00	8
5	MOTA	1566	N	CYS				80.819	18.530	6.155	1.00	20.00	7
•	MOTA	1567	CA	CYS				80.445	17.613	5.083	1.00	20.00	6
	ATOM	1568	СВ	CYS				79.413	18.255	4.148	1.00	20.00	6
	ATOM	1569	SG	CYS	В	270		77.824	18.654	4.905	1.00	20.00	16
	ATOM	1570	С	CYS				81.682	17.241	4.265	1.00	20.00	6
10	ATOM	1571	0	CYS				81.852	16.090	3.866	1.00	20.00	8
	ATOM	1572	N	ILE	В	271		82.541	18.226	4.012	1.00	20.00	. 7
	ATOM	1573	CA	ILE				83.751	18.000	3.229	1.00	20.00	6
	ATOM	1574	CB	ILE	В	271		84.436	19.339	2.903	1.00	20.00	6
	MOTA	1575	CG2	ILE	В	271		85.784	19.098	2.227	1.00	20.00	6
15	ATOM	1576		ILE				83.508	20.171	2.007	1.00	20.00	6
	ATOM	1577		ILE				83.962	21.607	1.815	1.00	20.00	6
	ATOM	1578	С	ILE				84.729	17.063	3.934	1.00	20.00	6
	ATOM	1579	0	ILE	В	271		85.300	16.174	3.304	1.00	20.00	8 .
	MOTA	1580	N	ILE	В	272		84.927	17.258	5.236	1.00	20.00	7
20	MOTA	1581	CA	ILE				85.820	16.382	5.987	1.00	20.00	6
	ATOM	1582	CB	ILE	В	272		85.902	16.790	7.471	1.00	20.00	6
	ATOM	1583	CG2	ILE	в	272		86.623	15.703	8.277	1.00	20.00	6
	ATOM	1584		ILE				86.646	18.120	7.606	1.00	20.00	6
	ATOM	1585	CD1	ILE	В	272		86.553	18.723	9.011	1.00	20.00	6
25	ATOM	1586	С	ILE	В	272		85.274	14.957	5.901	1.00	20.00	6
	ATOM	1587	0	ILE				86.021	14.003	5.679	1.00	20.00	8
	ATOM	1588	N	TYR	В	273		83.964	14.822	6.072	1.00	20.00	7
	ATOM	1589	CA	TYR	В	273		83.324	13.518	6.006	1.00	20:00	6
	MOTA	1590	CB	TYR	В	273	-	81.825	13.651	6.287	1.00	20.00	6
30	MOTA	.1591	CG	TYR	В	273		81.064	12.340	6.250	1.00	20.00	6
	ATOM	1592	CD1	TYR	В	273		80.806	11.690	5.041	1.00	20.00	6
	ATOM	1593	CE1	TYR	В	273		80.107	10.486	5.005	1.00	20.00	6 .
	ATOM	1594	CD2	TYR	В	273		80.601	11.750	7.427		20.00	6
	ATOM	1595	CE2	TYR	В	273		79.904	10.548	7.405	1.00	20.00	6
35	ATOM	1596	CZ	TYR	В	273		79.659	9.922	6.192		20.00	6
	ATOM	1597	OH	TYR	В	273		78.971	8.736	6.174		20.00	8
	MOTA	1598	С	TYR				83.550	12.897	4.632		20.00	6
	ATOM	1599	0	TYR				83.865	11.713	4.526		20.00	8
	MOTA	1600	N	GLN				83.402	13.705	3.586		20.00	7
40	MOTA	1601	CA	GLN				83.579	13.230	2.220		20.00	6
	ATOM	1602	CB	GLN	В	274		83.176	14.322	1.222		20.00	6
	ATOM	1603	CG	GLN				83.149	13.857	-0.230		20.00	6
	ATOM	1604	CD	GLN				82.558	14.898	-1.169		20.00	6
	MOTA	1605		GLN				82.108	15.961	-0.736		20.00	8
45	ATOM	1606		GLN				82.548		-2.462		20.00	7
	ATOM	1607	С	GLN				85.013	12.788	1.953		20.00	6
	MOTA	1608	0	GLN				85.239	11.818	1.233		20.00	. 8
	ATOM	1609	N	LEU				85.981	13.498	2.528		20.00	7
•	ATOM	1610	CA	LEU				87.389	13.143	2.333		20.00	6
50	ATOM	1611	CB	LEU				88.311	14.194	2.971		20.00	6
	ATOM	1612	CG	LEU				88.418	15.561	2.284		20.00	6
	MOTA	1613		LEU				89.325	16.481	3.088		20.00	6
	MOTA	1614		LEU				88.969	15.379	0.879		20.00	6
	ATOM	1615	С			275		87.697	11.779	2.940		20.00	6
55	ATOM	1616	0	LEU				88.430	10.981	2.354		20.00	8
	ATOM	1617	N	VAL				87.125	11.519	4.112		20.00	7
	MOTA	1618	CA	VAL				87.353	10.269	4.827		20.00	6
	ATOM	1619	CB	VAL				87.096	10.451	6.342		20.00	6
	ATOM	1620	CGI	VAL	В	2/6		87.376	9.148	7.082	1.00	20.00	6

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	ATOM	1621		VAL			87.973	11.580	6.891	1.00 20.00	6 6
	ATOM	1622	С	VAL			86.504	9.089	4.336	1.00 20.00	
	ATOM	1623	0	VAL			87.005	7.973	4.195	1.00 20.00	8
	MOTA	1624	N	ALA			85.222	9.337	4.090	1.00 20.00	7
5	MOTA	1625	CA	ALA			84.310		3.643	1.00 20.00	6
	MOTA	1626	CB	ALA			82.898	8.597	4.124	1.00 20.00	6
	ATOM	1627	С	ALA			84.315	8.115	2.130	1.00 20.00	6
	MOTA	1628	0	ALA	В	277	84.036	7.029	1.627	1.00 20.00	8
	MOTA	1629	N	GLY	В	278	84.632	9.180	1.405	1.00 20.00	7
10	MOTA	1630	CA	GLY	В	278	84.653	9.099	-0.041	1.00 20.00	6
	ATOM	1631	С	GLY	В	278	83.365	9.627	-0.644	1.00 20.00	6
	ATOM	1632	0	GLY	В	278	83.272	9.817	-1.860	1.00 20.00	8
	ATOM	1633	N	LEU	В	279	82.375	9.867	0.211	1.00 20.00	7
	ATOM	1634	CA	LEU	В	279	81.075	10.382	-0.219	1.00 20.00	6
15	ATOM	1635	CB	LEU			80.070	9.232	-0.375	1.00 20.00	6
10	ATOM	1636	CG	LEU			80,342	8.114	-1.385	1.00 20.00	6
	ATOM	1637		LEU			79.311	7.009	-1.191	1.00 20.00	6
	ATOM	1638		LEU			80.291	8.660	-2.804	1.00 20.00	6
	ATOM	1639	C	LEU			80.522	11.369	0.812	1.00 20.00	6
20		1640	Ö	LEU			80.750	11.218	2.007	1.00 20.00	8
-20	ATOM	1641	И	PRO			79.787	12.395	0.361	1.00 20.00	7
	ATOM	1642	CD.	PRO			79.403	12.730	-1.020	1.00 20.00	6
	ATOM		CA	PRO			79.230	13.361	1.314	1.00 20.00	6
	MOTA	1643		PRO			78.569	14.397	0.407	1.00 20.00	6
0.5	MOTA	1644	CB	PRO			78.191	13.598	-0.802	1.00 20.00	6
25	MOTA	1645	CG				78.242	12.662	2.262	1.00 20.00	6
	MOTA	1646	C			280	77.666	11.633	1.913	1.00 20.00	8
	ATOM	1647	0	PRO					3.470	1.00 20.00	7
	MOTA	1648	N	PRO			78.035	13.220	3.859	1.00 20.00	6
	MOTA	1649	CD	PRO			78.571	14.535		1.00 20.00	6
30	MOTA	1650	CA	PRO			77.145	12.701	4.520	1.00 20.00	6
	MOTA	1651	CB	PRO			77.262	13.746	5.634	1.00 20.00	6
	MOTA	1652	CG			281	78.546	14.450	5.344	1.00 20.00	6
	MOTA	1653	С	PRO			75.679	12.485	4.142	1.00 20.00	8
	ATOM	1654	0	PRO			75.094	11.441	4.442	1.00 20.00	7
35	MOTA	1655	N			282	75.088	13.487	3.504	1.00 20.00	
	ATOM	1656	CA			282	73.686	13.427	3.123	1.00 20.00	6
	MOTA	. 1657	СВ			282	73.006	14.734	3.531	1.00 20.00	
	ATOM	1658	CG			282	73.300	15.146	4.947	1.00 20.00	
	ATOM	1659		PHE			72.624	14.560	6.013	1.00 20.00	6 6
40 /		1660		PHE			74.295	16.085	5.218		6
	MOTA	1661		PHE			72.934	14.902	7.331	1.00 20.00	6
	ATOM	1662		PHE			74.613	16.433	6.530		6
	MOTA	1663	CZ			282	73.930	15.840	7.591	1.00 20.00	6
	ATOM	1664	С			282	73.527	13.191	1.628	1.00 20.00	
45	MOTA	1665	0	PHE				14.079		1.00 20.00	
	MOTA	1666	N			283	73.080	11.994	1.267	1.00 20.00	7
	MOTA	1667	CA			283	72.888	11.635	-0.134	1.00 20.00	6
	MOTA	1668	CB	ARG			73.931	10.598	-0.559	1.00 20.00	6
	ATOM	1669	CG			283	75.358	10.928	-0.151	1.00 20.00	6
50	ATOM	1670	CD			283	76.326	9.883	-0.687	1.00 20.00	6
	ATOM	1671	NE			283	76.054	8.555	-0.142	1.00 20.00	7
	ATOM	1672	CZ			283	76.404	8.159	1.077	1.00 20.00	6
	ATOM	1673	NH1	ARG	В	283	77.047	8.986	1.893	1.00 20.00	7
	ATOM	1674				283	76.108	6.933	1.484	1.00 20.00	7
55	ATOM	1675	С			283	71.493	11.046	-0.331	1.00 20.00	6
	ATOM	1676	Ο.			283	70.957	10.391	0.563	1.00 20.00	8
	ATOM	1677	N			284	70.911	11.276	-1.502	1.00 20.00	7
	ATOM	1678	CA			284	69.579	10.755	-1.796	1.00 20.00	6
	ATOM	1679	CB	ALA	В	284	68.532	11.484	-0.961	1.00 20.00	6

	ATOM	1680	С	ALA	В	284	69.278	10.921	-3.273	1.00 20.	00	6
	MOTA	1681	0	ALA	В	284	70.007	11.611	-3.984	1.00 20.		8
	ATOM	1682	N	GLY	В	285	68.191	10.299	-3.722	1.00 20.		7
	ATOM	1683	CA	GLY	В	285	67.807	10.360	-5.122	1.00 20.	00	6
5	ATOM	1684	С	GLY	В	285	67.561	11.737	-5.707	1.00 20.		6
	ATOM	1685	0			285	67.775	11.955	-6.899	1.00 20.		8
	ATOM	1686	N	ASN	В	286	67.089	12.673	-4.892	1.00 20.		7
	ATOM	1687	CA	ASN			66.835	14.018	-5.386	1.00 20.		6
	ATOM	1688	CB	ASN	В	286	65.403	14.137	-5.930	1.00 20.		6
10	ATOM	1689	CG	ASN	В	286	64.342	13.825	-4.885	1.00 20.0		6
	ATOM	1690		ASN			64.292	14.450	-3.826	1.00 20.0		8
	ATOM	1691	ND2	ASN	В	286	63.477		-5.190	1.00 20.0		7
	ATOM	1692	С	ASN			67.076	15.042	-4.291	1.00 20.0		6
	ATOM	1693	0	ASN			67.368	14.682	-3.152	1.00 20.0		8
15	ATOM	1694	N	GLU			66.955	16.317	-4.636	1.00 20.0		7
	ATOM	1695	CA	GLU			67.185	17.377	-3.669	1.00 20.0		6
_	ATOM	1696	СВ	GLU			67.181	18.738	-4.365	1.00 20.0		6
•	ATOM	1697	CG	GLU			68.537	19.095	-4.944	1.00 20.0		6
	ATOM	1698	CD	GLU			68.524	20.385	-5.735	1.00 20.0		6
20	ATOM	1699		GLU			67.911	21.371	-5.267	1.00 20.0		8
_,	ATOM -	1700		GLU			69.144	20.410	-6.823	1.00 20.0		8
	ATOM	1701	C	GLU			66.225	17.394	-2.492	1.00 20.0		6
	ATOM	1702	ō	GLU			66.658	17.554	-1.354	1.00 20.0		8
	ATOM	1703	Ņ	TYR			64.932	17.233	-2.753	1.00 20.0		7
25	ATOM	1704	CA	TYR			63.955	17.239	-1.670	1.00 20.0		6
	ATOM	1705	СВ	TYR			62.553	16.899	-2.184	1.00 20.0		6
	ATOM	1706	CG	TYR			61.530	16.780	-1.070	1.00 20.0		6
	ATOM	1707		TYR			60.984	17.917	-0.470	1.00 20.0		6
	ATOM	1708		TYR			60.090	17.814	0.600	1.00 20.0		6
30	ATOM	1709		TYR			61.154	15.529	-0.573	1.00 20.0		6
•	ATOM	1710	CE2	TYR			60.265	15.414	0.498	1.00 20.0		6
	ATOM	1711	CZ	TYR			59.740	16.561	1.078	1.00 20.0		6
	ATOM	1712	ОН	TYR			58.884	16.454	2.149	1.00 20.0		8
	ATOM	1713	C	TYR			64.337	16.238	-0.587	1.00 20.0		6
35	ATOM	1714	ō	TYR			64.254	16.545	0.598	1.00 20.0		8
	ATOM	1715	N	LEU			64.750	15.041	-1.001	1.00 20.0		7
	ATOM	1716	CA	LEU			65.137	13.989	-0.064	1.00 20.0		6
	ATOM	1717	СВ	LEU			65.283	12.649	-0.797	1.00 20.0		6
	ATOM	1718	CG	LEU			63.984	11.985	-1.274	1.00 20.0		6
40	ATOM	1719	CD1	LEU			64.314	10.802	-2.179	1.00 20.0		6
	MOTA	1720		LEU			63.160	11.530	-0.068	1.00 20.0		6
	ATOM	1721	C	LEU			66.431	14.310	0.685	1.00 20.0		6
	ATOM	1722	0	LEU			66.604	13.914	1.840	1.00 20.0	-	8
	ATOM	1723	N	ILE			67.340	15.017	0.025	1.00 20.0		7
45	ATOM	1724	CA	ILE				15.390		1.00 20.0	-	6
	ATOM	1725	СВ	ILE	В	290	69.583	15.985	-0.366	1.00 20.0		6
	ATOM	1726		ILE			70.778	16.609	0.359	1.00 20.0		6
	ATOM	1727		ILE			70.046	14.887	-1.330	1.00 20.0		6
	ATOM	1728		ILE			70.844	15.398	-2.518	1.00 20.0		6
50	ATOM	1729	C .	ILE			68.307	16.424	1.743	1.00 20.0		6
	ATOM	1730	0	ILE			68.807	16.317	2.862	1.00 20.0		8
	ATOM	1731	N	PHE			67.491	17.420	1.411	1.00 20.0	-	7
	ATOM	1732	CA	PHE			67.143	18.462	2.372	1.00 20.0		6
	ATOM	1733	CB	PHE			66.222	19.502	1.731	1.00 20.0		6
55	ATOM	1734	CG	PHE			66.869	20.289	0.628	1.00 20.0		6
	ATOM	1735		PHE			68.255	20.420	0.568	1.00 20.0		6
	ATOM	1736		PHE			66.094	20.931	-0.332	1.00 20.0		6
	ATOM	1737		PHE			68.859	21.182	-0.435	1.00 20.0		6
	ATOM	1738		PHE			66.690	21.697	-1.340	1.00 20.0		6
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	ATOM	1739	CZ	PHE	В	291		68.074	21.822	-1.390	1.00 20.00	. 6
	ATOM	1740	C			291		66.453	17.848	3.576	1.00 20.00	
	ATOM	1741	ō			291		66.664	18.262	4.718	1.00 20.00	
	ATOM	1742	N			292		65.629	16.847	3.303	1.00 20.00	
5	ATOM	1743	CA			292		64.887	16.154	4.341	1.00 20.00	
•	ATOM	1744	CB			292		64.006	15.090	3.687	1.00 20.00	
	ATOM	1745	CG			292		62.953	14.486	4.572	1.00 20.00	
	ATOM	1746	CD			292		61.895	13.750	3.763	1.00 20.00	
		1747		GLN				62.208	12.835	2.997		
10	ATOM ATOM	1748		GLN				60.637	14.155		1.00 20.00	
10								65.865		3.924		
	ATOM	1749	C			292 292		65.689	15.522	5.329	1.00 20.00	
•	ATOM	1750 1751	0						15.630	6.540	1.00 20.00	-
	MOTA		N			293 293		66.907	14.875	4.812	1.00 20.00	7
1.5	ATOM	1752	CA					67.898	14.244	5.683	1.00 20.00	6
15	ATOM	1753	CB			293		68.850	13.372	4.865	1.00 20.00	6
	ATOM	1754	CG			293	•	68.197	12.135	4.278	1.00 20.00	6
	ATOM	1755	·CD			293		69.217	11.260	3.554	1.00 20.00	6
	ATOM	1756	CE			293		68.575	9.972	3.051	1.00 20.00	6
20	ATOM	1757	NZ			293		69.553	9.099	2.339	1.00 20.00	7 -
20	ATOM	1758	C			293		68.698	15.287	6.468	1.00 20.00	6
	ATOM	1759	0			293		69.044	15.074	7.634	1.00 20.00	8
	ATOM	1760	N	ILE				68.989	16.411	5.827	1.00 20.00	7.
	ATOM	1761	CA			294		69.745	17.480	6.472 5.474	1.00 20.00	6
25	ATOM	1762 1763	CB	ILE				70.026	18.632 19.881		1.00 20.00	6
23	ATOM	1763		ILE				70.489		6.223	1.00 20.00	6
	ATOM ATOM	1765		ILE				71.070 71.266	18.178 19.159	4.443	1.00 20.00	6 6
	ATOM	1766	CDI	ILE				69.035	18.045	7.712	1.00 20.00	6
	ATOM	1767	0	ILE				69.618	18.091	8.798	1.00 20.00	8
30	MOTA	1768	N	ILE				67.783		7.564	1.00 20.00	7
50	ATOM	1769	CA	ILE				67.068	19.037	8.707	1.00 20.00	6
	ATOM	1770	CB			295		65.710	19.647	8.300	1.00 20.00	6
	MOTA	1771		ILE				65.927	20.749	7.265	1.00 20.00	6
	ATOM	1772		ILE				64.784	18.559	7.762	1.00 20.00	6
35	ATOM	1773		ILE				63.356	19.037	7.558	1.00 20.00	6
7,5	MOTA	1774	C	ILE				66.831	18.045	9.842	1.00 20.00	6
	ATOM	1775	ŏ	ILE				66.540	18.447	10.967	1.00 20.00	8
	ATOM	1776	N	LYS				66.956	16.753	9.550	1.00 20.00	7
	ATOM	1777	CA	LYS				66.765	15.724	10.569	1.00 20.00	6
40	ATOM	1778	CB	LYS				65.907	14.576	10.019	1.00 20.00	6
	ATOM	1779	CG	LYS				64.535	15.010	9.538	1.00 20.00	6
	ATOM	1780	CD	LYS				63.739	13.851	8.951	1.00 20.00	6
	ATOM	1781	CE	LYS				63.296	12.873	10.025	1.00 20.00	6
	MOTA	1782	NZ	LYS	В	296		62.375	11.828	9.482	1.00 20.00	7
45	ATOM	1783	C	LYS	В	296		68.116	15.176	11.018	1.00 20.00	6
	MOTA	1784	0	LYS				68.178	14.261	11.838	1.00 20.00	8
	MOTA	1785	N	LEU				69.190	15.746	10.474	1.00 20.00	7
	MOTA	1786	CA	LEU	В	297		70.551	15.320	10.791	1.00 20.00	6
	ATOM	1787	СВ	LEU				70.911	15.680	12.236	1.00 20.00	6
50	ATOM	1788	CG	LEU				72.398	15.538	12.585	1.00 20.00	6
	MOTA	1789	CD1	LEU	В	297		73.215	16.555	11.771	1.00 20.00	6
	MOTA	1790		LEU				72.605	15.762	14.076	1.00 20.00	6
	ATOM	1791	С	LEU	В	297		70.635	13.810	10.592	1.00 20.00	6
	ATOM	1792	0	LEU	В	297		71.150	13.080	11.434	1.00 20.00	8
55	ATOM	1793	N	GLU	В	298		70.128	13.351	9.456	1.00 20.00	7
	ATOM	1794	CA	GLU				70.115	11.934	9.148	1.00 20.00	6
	MOTA	1795	CB	GLU	В	298		68.817	11.597	8.416	1.00 20.00	6
	ATOM	1796	CG	GLU				68.568	10.123	8.233	1.00 20.00	6
	MOTA	1797	CD	GLU	В	298		67.254	9.858	7.535	1.00 20.00	6

	AȚOM ATOM ATOM ATOM	1798 1799 1800 1801		GLU GLU	B 298 B 298 B 298 B 298	66.214 67.261 71.309 71.310	10.331 9.185 11.446 11.523	8.043 6.484 8.332 7.104	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	8 8 6 8
5	ATOM ATOM ATOM	1802 1803 1804	N CA CB	TYR TYR	B 299 B 299 B 299	72.325 73.519 74.444	10.946 10.405 11.521	9.027 8.390 7.880	1.00 20.00 1.00 20.00 1.00 20.00	7 6 6
10	ATOM ATOM ATOM ATOM ATOM	1805 1806 1807 1808 1809	CE1 CD2	TYR TYR TYR	B 299 B 299 B 299 B 299 B 299	75.330 74.796 75.589 76.692 77.499	12.130 12.962 13.482 11.833 12.352	8.953 9.935 10.951 9.013 10.032	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 6 6
15	ATOM ATOM ATOM ATOM ATOM	1810 1811 1812 1813 1814	CZ OH C	TYR TYR TYR TYR	B 299 B 299 B 299 B 299 B 300	76.935 77.701 74.245 73.913 75.229	13.173 13.687 9.600 9.688 8.808	10.995 12.006 9.456 10.631 9.052	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 8 6 8
20	ATOM ATOM ATOM ATOM ATOM	1815 1816 1817 1818 1819	CA CB CG OD1	ASP ASP ASP	300 300 300 300 300 300	75.991 75.291 74.898 75.806 73.681	8.030 6.700 5.968 5.594 5.771	10.016 10.304 9.048 8.274 8.832	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 8 8
25	ATOM ATOM ATOM ATOM ATOM	1820 1821 1822 1823 1824	C O .N CA CB	ASP ASP PHE PHE	300 300 301 301 301 301	77.397 77.651 78.307 79.695 80.655	7.799 7.976 7.417 7.186 7.664	9.488 8.297 10.378 9.996 11.093	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 8 7 6 6
30	MOTA MOTA MOTA	1825 1826 1827 1828 1829	CG CD1 CD2 CE1		301 301 301 301 301	80.488 79.493 81.346 79.352 81.214	9.103 9.487 10.075 10.823 11.408	11.481 12.370 10.970 12.750 11.342	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 6 6
35	ATOM ATOM ATOM ATOM	1830 1831 1832 1833	CZ C O N	PHE : PHE : PHE :	301 301 301 302	80.215 80.009 79.506 80.842	11.783 5.722 4.839 5.440	12.235 9.744 10.442 8.732	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 8 7
40	ATOM ATOM ATOM ATOM ATOM	1834 1835 1836 1837 1838	CD CA CB CG	PRO PRO PRO	B 302 B 302 B 302 B 302 B 302	81.330 81.191 81.838 82.425 82.168	6.316 4.044 4.105 5.479 3.629	7.654 8.466 7.084 7.046 9.569	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 6 6
45	ATOM ATOM ATOM ATOM ATOM	1839 1840 1841 1842 1843	O N CA CB C	ALA : ALA : ALA :	3 302 3 303 3 303 3 303 3 303	82.887 82.185 83.052 82.993 84.513	4.469 2.345 1.836 0.310 2.294	10.111 9.908 10.968 10.987 10.939	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	8 7 6 6
50	MOTA MOTA MOTA MOTA	1844 1845 1846 1847	O N CA CB	ALA :	3 303 3 304 3 304 3 304	85.078 85.121 86.527 86.971	2.637 2.306 2.684 2.423	11.979 9.756 9.605 8.165	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	8 7 6 6
. 55	ATOM ATOM ATOM ATOM	1848 1849 1850 1851 1852	C O N CA CB	ALA : PHE : PHE :	3 304 3 304 3 305 3 305 3 305	86.894 87.983 85.985 86.183 84.822	4.119 4.367 5.053 6.473 7.115	10.001 10.520 9.742 10.034 10.312	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 8 7 6 6
	ATOM ATOM ATOM ATOM ATOM	1852 1853 1854 1855 1856	CG CD1 CD2		305 305 305	84.705 85.303 84.003 85.202	8.522 9.572 8.800 10.881	9.815 10.502 8.646 10.033	1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00	6 6 6

	ATOM	1857	CE2	PHE	В	305		83.896	10.106	8.167	1.00 20.00	б
	MOTA	1858	CZ	PHE	В	305		84.496	11.147	8.862	1.00 20.00	
	ATOM	1859	С	PHE	В	305		87.153	6.789	11.182	1.00 20.00	
	ATOM	1860	0	PHE	В	305		86.964	6.342	12.312	1.00 20.00	
5	ATOM	1861	N	PHE	В	306		88.190	7.565	10.883	1.00 20.00	
	ATOM	1862	CA	PHE	В	306		89.176	7.945	11.894	1.00 20.00	6
	ATOM	1863	CB	PHE	В	306		90.179	8.936	11.295	1.00 20.00	
•	MOTA	1864	CG	PHE	В	306		90.695	8.531	9.940	1.00 20.00	
	ATOM	1865	CD1	PHE	В	306		91.292	7.284	9.747	1.00 20.00	
10	ATOM	1866		PHE		306		90.588	9.395	8.853	1.00 20.00	
	ATOM	1867	CE1	PHE	В	306		91.774	6.906	8.490	1.00 20.00	
	ATOM	1868	CE2	PHE	В	306		91.067	9.027	7.590	1.00 20.00	
	ATOM	1869	CZ	PHE	В	306		91.662	7.780	7.408	1.00 20.00	
	ATOM	1870	С	PHE	В	306		88.445	8.575	13.086	1.00 20.00	
15	ATOM	1871	0	PHE				87.731	9.566	12.936	1.00 20.00	
	ATOM	1872	N	PRO				88.614	7.995	14.288	1.00 20.00	
	ATOM	1873	CD	PRO				89.482	6.834	14.555	1.00 20.00	
	ATOM	1874	CA	PRO				87.983	8.459	15.530	1.00 20.00	
	ATOM	1875	СВ	PRO		307		88.748	7.691	16.606	1.00 20.00	6
20	ATOM	1876	CG	PRO				89.018	6.388	15.928	1.00 20.00	6
	ATOM	1877	C	PRO			-	87.986	9.965	15.784	1.00 20.00	6
	ATOM	1878	ō	PRO				86.936	10.565	16.025		
	ATOM~	1879	N	LYS				89.162	10.575	15.745	1.00 20.00	7
	ATOM	1880	CA	LYS				89.260	12.004	15.992	1.00 20.00	6
25	ATOM	1881	СВ	LYS				90.728		16.149	1.00 20.00	6
	ATOM	1882	CG	LYS				91.338	11.805	17.410	1.00 20.00	6
,	ATOM	1883	CD	LYS				92.806	12.140	17.591	1.00 20.00	6
	ATOM	1884	CE	LYS		•		93.339	11.457	18.847	1.00 20.00	6
	ATOM	1885	NZ	LYS				94.816	11.573	18.985	1.00 20.00	7
30	ATOM	1886	C	LYS				88.572	12.808	14.894	1.00 20.00	6
	ATOM	1887	ō	LYS		308		87.985	13.855	15.167	1.00 20.00	8
	ATOM	1888	N	ALA				88.629	12.318	13.659	1.00 20.00	7
	ATOM	1889	CA	ALA				87.967	13.011	12.557	1.00 20.00	6
	ATOM	1890	СВ	ALA		309		88.328	12.369	11.231	1.00 20.00	6
35	ATOM	1891	C	ALA				86.460	12.936	12.787	1.00 20.00	6
	ATOM	1892	ō	ALA		309		85.735	13.903	12.552	1.00 20.00	8
	ATOM	1893	N	ARG		310		85.986	11.780	13.246	1.00 20.00	7
	ATOM	1894	CA	ARG				84.561	11.619	13.513	1.00 20.00	6
	ATOM	1895	СВ	ARG				84.246	10.194	13.979	1.00 20.00	6
40	ATOM	1896	CG	ARG		310		82.844	10.069	14.561	1.00 20.00	6
	ATOM	1897	CD	ARG				82.408	8.632	14.789	1.00 20.00	6
	ATOM	1898	NE	ARG	В	310		81.060	8.593	15.355	1.00 20.00	7
	MOTA	1899	CZ	ARG		310		80.259	7.532	15.328	1.00 20.00	6
	ATOM	1900	NH1	ARG				80.665	6.401	14.759	1.00 20.00	7
45	ATOM	1901	NH2	ARG	В	310		79.048	7.601	15.867	1.00 20.00	7
	ATOM	1902	С	ARG				84.110	12.613	14.583	1.00 20.00	6
	ATOM	1903	0	ARG				83.080	13.274	14.436	1.00 20.00	8
	ATOM	1904	N	ASP				84.876	12.707	15.666	1.00 20.00	7
	ATOM	1905	CA	ASP				84.535	13.629	16.740	1.00 20.00	6
50	ATOM	1906	СВ	ASP				85.574	13.555	17.864	1.00 20.00	6
	ATOM	1907	CG	ASP				85.260	14.505	19.006	1.00 20.00	6
	ATOM	1908		ASP				85.782	15.636	19.010	1.00 20.00	8
	ATOM	1909		ASP				84.480	14.124	19.901	1.00 20.00	8
	ATOM	1910	С	ASP				84.445	15.054	16.198	1.00 20.00	6
55	ATOM	1911	ŏ	ASP				83.539	15.800	16.564	1.00 20.00	8
	ATOM	1912	N	LEU				85.371	15.423	15.313	1.00 20.00	7
	ATOM	1913	CA	LEU				85.362	16.769	14.736	1.00 20.00	6
	ATOM	1914	CB	LEU				86.604	16.999	13.869	1.00 20.00	6
	ATOM	1915	CG	LEU				86.662	18.329	13.099	1.00 20.00	6
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ATOM
              1916
                    CD1 LEU B 312
                                         86.424 19.510
                                                          14.037
                                                                   1.00 20.00
                    CD2 LEU B 312
      ATOM
              1917
                                         88.018
                                                 18.450
                                                          12.414
                                                                   1.00 20.00
      ATOM
              1918
                    C
                         LEU B 312
                                         84.112
                                                 17.008
                                                          13.899
                                                                   1.00 20.00
                                                                                6
      MOTA
              1919
                    0
                         LEU B 312
                                         83.456
                                                 18.039
                                                          14.035
                                                                   1.00 20.00
                                                                                8
      ATOM
              1920
                         VAL B 313
                    N
                                         83.786
                                                 16.051
                                                          13.033
                                                                   1.00 20.00
      ATOM
                        VAL B 313
              1921
                    CA
                                         82.611
                                                 16.171
                                                          12.183
                                                                   1.00 20.00
                                                                                6
      ATOM
              1922
                    CB
                         VAL B 313
                                         82.464
                                                 14.942
                                                          11.255
                                                                   1.00 20.00
                                                                                6
      ATOM
              1923
                        VAL B 313
                    CG1
                                         81.121
                                                 14.973
                                                          10.551
                                                                   1.00 20.00
                                                                                6
      ATOM
              1924
                    CG2 VAL B 313
                                         83.595
                                                 14.935
                                                          10.228
                                                                   1.00 20.00
                                                                                6
      ATOM
             1925
                         VAL B 313
                    С
                                         81.354
                                                 16.315
                                                          13.036
                                                                   1.00 20.00
                                                                                6
      ATOM
             1926
                        VAL B 313
                    0
                                         80.467
                                                 17.111
                                                          12.716
                                                                   1.00 20.00
                                                                                8
      ATOM
             1927
                    N
                        GLU B 314
                                         81.282
                                                 15.559
                                                          14.129
                                                                   1.00 20.00
                                                                                7
      ATOM
             1928
                    CA
                        GLU B 314
                                         80.122
                                                 15.634
                                                          15.010
                                                                   1.00 20.00
                                                                                6
      ATOM
             1929
                    CB
                        GLU B 314
                                         80.191
                                                 14.545
                                                          16.084
                                                                   1.00 20.00
                                                                                6
 15
      MOTA
             1930
                        GLU B 314
                    CG
                                         80.160 13.131
                                                                   1.00 20.00
                                                          15.521
                                                                                6
      ATOM
             1931
                        GLU B 314
                    CD
                                         80.222
                                                 12.073
                                                          16.603
                                                                   1.00 20.00
                                                                                6
                    OE1 GLU B 314
      ATOM
             1932
                                         81.033
                                                 12.227
                                                          17.542
                                                                   1.00 20.00
                                                                                8
      ATOM
             1933
                    OE2
                        GLU B 314
                                        79.469
                                                 11.081
                                                                  1.00 20.00
                                                          16.512
                                                                                8
      MOTA
             1934
                    С
                        GLU B 314
                                         80.035
                                                 17.005
                                                          15.664
                                                                   1.00 20.00
                                                                                6
 20
      MOTA
             1935
                        GLU B 314
                    0
                                         78.960
                                                 17.443
                                                          16.059
                                                                  1.00 20.00
      ATOM
             1936
                        LYS B 315
                   N
                                        81.165
                                                 17.690
                                                          15.776
                                                                  1.00 20.00
                                                                                7
      ATOM
             1937
                    CA
                        LYS B 315
                                        81.154
                                                 19.010
                                                          16.383
                                                                  1.00 20.00
                                                                                6
      ATOM
             1938
                        LYS B 315
                    CB
                                        82.448
                                                 19.240
                                                          17.168
                                                                  1.00 20.00
                                                                                6
      MOTA
             1939
                   CG
                        LYS B 315
                                        82.460
                                                 18.478
                                                          18.493
                                                                  1.00 20.00
                                                                                б
     ATOM
             1940
                   CD
                        LYS B 315
                                        83.803
                                                 18.529
                                                         19.198
                                                                  1.00 20.00
                                                                                6
                        LYS B 315
     MOTA
             1941
                   CE
                                        83.749
                                                 17.825
                                                         20.552
                                                                  1.00 20.00
                                                                                6
     MOTA
             1942
                        LYS B 315
                   ΝZ
                                        82.829
                                                 18.505
                                                         21.506
                                                                  1.00 20.00
                                                                               7
     ATOM
             1943
                   C
                        LYS B 315
                                        80.934
                                                 20.104
                                                         15.343
                                                                  1.00 20.00
                                                                                6
     ATOM
             1944
                        LYS B 315
                   0
                                        80.855
                                                 21.282
                                                         15.686
                                                                  1.00 20.00
30
     ATOM
             1945
                        LEU B 316
                   N
                                        80.819
                                                 19.706
                                                         14.075
                                                                  1.00 20.00
     ATOM
             1946
                       LEU B 316
                   CA
                                        80.577
                                                 20.649
                                                         12.979
                                                                  1.00 20.00
                                                                               6
     ATOM
             1947
                   CB
                       LEU B 316
                                        81.608
                                                 20.450
                                                         11.863
                                                                  1.00 20.00
                                                                               6
     ATOM
             1948
                   CG
                       LEU B 316
                                        83.044
                                                20.833
                                                         12.240
                                                                  1.00 20.00
                                                                               6
     MOTA
             1949
                   CD1 LEU B 316
                                        84.011
                                                20.365
                                                         11.156
                                                                  1.00 20.00
                                                                               6
                   CD2 LEU B 316
35
     MOTA
             1950
                                        83.124
                                                22.351
                                                         12.434
                                                                  1.00 20.00
                                                                               6
     MOTA
             1951
                   С
                        LEU B 316
                                        79.164
                                                20.469
                                                         12.415
                                                                  1.00 20.00
                                                                               6
     ATOM
             1952
                   0
                        LEU B 316
                                        78.464
                                                21.448
                                                         12.148
                                                                  1.00 20.00
     ATOM
             1953
                       LEU B 317
                   N
                                        78.746
                                                19.220
                                                         12.230
                                                                  1.00 20.00
                                                                               7
     ATOM
             1954
                       LEU B 317
                   CA
                                        77.403
                                                18.962
                                                                  1.00 20.00
                                                         11.721
                                                                               6
40
     ATOM
             1955
                   CB
                       LEU B 317
                                        77.343
                                                17.605
                                                         11.012
                                                                  1.00 20.00
                                                                               6
     ATOM
             1956
                   CG
                       LEU B 317
                                        78.335
                                                17.445
                                                          9.852
                                                                  1.00 20.00
                                                                               6
     ATOM
            1957
                   CD1 LEU B 317
                                        78.091
                                                16.111
                                                          9.143
                                                                  1.00 20.00
                                                                               6
     ATOM
            1958
                   CD2 LEU B 317
                                        78.182
                                                18.603
                                                          8.866
                                                                  1.00 20.00
                                                                               6
     ATOM
            1959
                       LEU B 317
                   С
                                       76.435
                                                19.000
                                                         12.899
                                                                  1.00 20.00
                                                                               6
45
     ATOM
            1960
                   0
                       LEU B 317
                                       75.979
                                                17.966
                                                         13.398
                                                                  1.00 20.00
                                                                               8
     ATOM
            1961
                                        76.156
                   Ν
                       VAL B 318
                                                20.215
                                                         13.354
                                                                  1.00 20.00
                                                                               7
     ATOM
            1962
                       VAL B 318
                   CA
                                       75.251
                                                20.451
                                                         14.467
                                                                  1.00 20.00
                                                                               6
     ATOM
            1963
                   CB
                       VAL B 318
                                       75.981
                                                21.164
                                                                  1.00 20.00
                                                         15.625
                                                                               6
                   CG1 VAL B 318
     ATOM
            1964
                                       75.007
                                                21.461
                                                         16.759
                                                                  1.00 20.00
                                                                               6
50
     ATOM
            1965
                  CG2 VAL B 318
                                       77.136
                                                20.300
                                                         16.115
                                                                  1.00 20.00
                                                                               6
     ATOM
            1966
                   C
                       VAL B 318
                                       74.140
                                                21.344
                                                         13.936
                                                                  1.00 20.00
     MOTA
            1967
                                     74.410
                   0
                       VAL B 318
                                                22.386
                                                        13.333
                                                                 1.00 20.00
                                                                               8
     ATOM
            1968
                   N
                       LEU B 319
                                       72.892
                                                20.941
                                                        14.153
                                                                 1.00 20.00
                                                                               7
    MOTA
            1969
                   CA
                       LEU B 319
                                       71.758
                                                21.717
                                                        13.663
                                                                 1.00 20.00
55
    ATOM
            1970
                  CB
                       LEU B 319
                                       70.444
                                                21.056
                                                        14.093
                                                                 1.00 20.00
    ATOM
            1971
                       LEU B 319
                  CG
                                       70.211
                                                19.647
                                                        13.533
                                                                 1.00 20.00
                                                                               6
    ATOM
            1972
                  CD1 LEU B 319
                                       68.883
                                                19.098
                                                        14.060
                                                                 1.00 20.00
                                                                               б
    ATOM
            1973
                  CD2 LEU B 319
                                       70.211
                                                19.688
                                                        12.000
                                                                 1.00 20.00
                                                                              6
    ATOM
            1974
                       LEU B 319
                                       71.794
                                                23.173
                                                        14.119
                                                                 1.00 20.00
```

						_		24.082	13.317	1.00 20.0	0	В
	ATOM	1975		LEU B		/	1.591	23.394	15.405	1.00 20.0		7
	MOTA	1976		ASP B			2.052		15.958	1.00 20.0		6
	ATOM	1977	CA	ASP B	320		2.119	24.745		1.00 20.0	-	6 [.]
	ATOM	1978	CB	ASP B	320		2.091	24.687	17.490		-	
5	ATOM	1979		ASP B			2.058	26.061	18.129	1.00 20.0		6
,		1980	OD1	ASP B	320	7	2.506	27.036	17.492	1.00 20.0		8
	MOTA	1981	002	ASP B	320		1.595	26.166	19.284	1.00 20.0		8
	MOTA			ASP B	320		3.415	25.419	15.492	1.00 20.0	0	6
	MOTA	1982		ASP B			4.496	25.089	15.965	1.00 20.0	0	8
	MOTA	1983	0	ASP B	320		3.294	26.372	14.576	1.00 20.0	0	7
10	MOTA	1984	N	ALA B	321		4.450	27.078	14.028	1.00 20.0		6
	MOTA	1985	CA	ALA B					13.006	1.00 20.0		6
	MOTA	1986	CB	ALA B			3.982	28.109		1.00 20.0		6
	MOTA	1987	С	ALA B	321		5.359	27747	15.065			Q
	ATOM	1988	0	ALA B	321	7	6.535	27.992	14.790	1.00 20.0		7
15	ATOM	1989	N	THR B	322	7	4.829	28.035	16.252	1.00 20.0		
13		1990	CA	THR B		7	5.631	28.681	17.292	1.00 20.0		6
	MOTA	1991	CB	THR B	322	7	4.755	29.491	18.271	1.00 20.0		6
	MOTA			THR B			3.879	28.605	18.973	1.00 20.0		8
	MOTA	1992	OG1		322		3.928	30.527	17.519	1.00 20.	00	6
	MOTA	1993	CG2				6.437	27.684	18.108	1.00 20.	00	6
20	MOTA	1994	С		322			28.071	19.019	1.00 20.	00	8
	MOTA	1995	0	THR B			7.166	26.401	17.786	1.00 20.		7
	ATOM	1996	N	LYS B			6.312		18.517	1.00 20.		6
	ATOM	1997	CA	LYS B			77.048	25.378		1.00 20.		6
	ATOM	1998	CB	LYS B			76.080	24.378	19.155	1.00 20.		6
25	ATOM	1999	CG	LYS B	323		75.180	24.992	20.209			6
23	ATOM	2000	CD	LYS B		•	74.356	23.931	20.924	1.00 20.		
	ATOM	2001	CE	LÝS B		•	73.406	24.574	21.927	1.00 20.		6
		2002	NZ	LYS B			74.144	25.514	22.818	1.00 20.		7
	ATOM		C				78.066	24.631	17.664	1.00 20.	00	6
	MOTA	2003		LYS B			78.520	23.557	18.040	1.00 20.		8
30	MOTA	2004	0				78.427	25.195	16.517	1.00 20.	00	7
	MOTA	2005	N	ARG B			79.408	24.545	15.656	1.00 20.		6
	MOTA	2006	CA	ARG B				24.834	14.186	1.00 20.		6
	MOTA	2007	CB	ARG B			79.108	24.034	13.728	1.00 20.		6
	MOTA	2008	CG	ARG B			77.824		12.297	1.00 20.		6
35	MOTA	2009	CD	ARG B			77.468		12.257	1.00 20.		7
	MOTA	2010	NE	ARG B	324		76.060			1.00 20.		6
	MOTA	2011	CZ	ARG B	324		75.277		11.233	1.00 20.		7
	ATOM	2012	NH1	ARG B	324		75.764		10.523	1.00 20		7
	ATOM	2013		ARG B			73.992		11.140			6
40	ATOM	2014	С	ARG B			80.811		16.008	1.00 20		
40	ATOM	2015		ARG B			81.070	26.212	16.131	1.00 20	.00	8
		2016		LEU B			81.711	24.049	16.180	1.00 20	.00	7
	MOTA	.2017		LEU E			83.090		16.520	1.00 20	.00 ,	6
	ATOM			LEU E			83.913		16.550	1.00 20	.00	6
	MOTA	2018		LEU E	225		85.274		17.241	1.00 20	.00	6
45	MOTA	2019	CG	LEU E	323		85.093			1.00 20	.00	6
	MOTA	2020		L LEU E	3 323		85.922				.00	6
	MOTA	2021		2 LEU E			03.322	25.310				6
	ATOM	2022	C	LEU E			83.656	_			.00	8
	MOTA	2023	0	LEU E			83.649					7
50	ATOM	2024	N	GLY I			84.139					6
	ATOM	2025		GLY E			84.697					6
	ATOM	2026			3 326		83.857				.00	
	MOTA	2027			3 326		84.369					8
	ATOM	2028			3 327		82.575	5 28.632				7
		2029			в 327		81.71		15.200			6
55	ATOM			CVC	B 327		80.23			1.00 20		6
	MOTA	2030			B 327		79.53			1.00 20		
	MOTA	2031		CIS	B 327		81.97			1.00 20	.00	6
	ATOM	2032		CYS	D 321						.00	8
	MOTA	203	3 0	CYS :	в 327		82.56	J JU.41(	,			

					_								
	ATOM	2034	N	GLU				81.523	32.005	16.178		20.00	7
	MOTA	2035	CA			328		81.714	33.052	17.167		20.00	6
	ATOM	2036	CB	GLU				81.087	34.348	16.632		20.00	6
_	ATOM	2037	CG	GLU		328		81.734	34.772	15.300		20.00	
5	ATOM	2038	CD	GLU				80.962	35.842	14.539	1.00	20.00	6
	ATOM	2039		GLU		328		79.738	35.676	14.343	1.00	20.00	8
	ATOM	2040	OE2	GLU	В	328		81.588	36.840	14.116	1.00	20.00	8
	ATOM	2041	С	GLU	В	328		81.187	32.701	18.560	1.00	20.00	6
	ATOM	2042	0	GLU	В	.328		81.850	32.983	.19.562	1.00	20.00	8
10	ATOM	2043	N	GLU	В	329		80.016	32.073	18.631	1.00	20.00	7
	ATOM	2044	CA	GLU	В	329		79.449	31.714	19.926		20.00	6
	ATOM	2045	CB	GLU		329		77.991	31.263	19.782		20.00	6
	ATOM	2046	CG	GLU				77.028	32.355	19.315		20.00	6
	ATOM	2047	CD	GLU				77.055	32.575	17.813		20.00	6
15	ATOM	2048		GLU				77.859	31.910	17.120		20.00	8
	ATOM	2049		GLU		329		76.267	33.413	17.323		20.00	8
	ATOM	2050	C	GLU				80.264	30.616	20.605		20.00	6
	ATOM	2051	Ö	GLU				80.182	30.436	21.819		20.00	8
	ATOM	2052	N	MET				81.040	29.878	19.816		20.00	7
20		2052	CA	MET				81.880	28.813	20.354			
20	ATOM											20.00	6
	ATOM	2054	CB	MET				81.872 80.552	27.600 26.822	19.419		20.00	6
	ATOM	2055	CG	MET						19.436		20.00	6
	ATOM	2056	SD	MET				80.117	26.254	21.104		20.00	16
05	MOTA	2057	CE	MET	_			81.265	24.895	21.311		20.00	6
25	ATOM	2058	C	MET		330		83.302	29.330	20.547		20.00	6
	ATOM	2059	0	MET		330		84.236	28.564	20.754		20.00	8
	MOTA	2060	N .	GLU		331	•	83.443	30.647	20.471		20.00	7
	ATOM	2061	CA	GLU	-	331		84.716	31.338	20.656		20.00	6
	ATOM	2062	CB	GLU				85.357	30.921	21.987		20.00	6
30	MOTA	2063	CG	GLU				84.371	30.886	23.163		20.00	6
	ATOM	2064	CD	GLU		331		83.478	32.127	23.270		20.00	6
	ATOM	2065		GLU				82.483	32.064	24.021	1.00	20.00	8
	ATOM	2066	OE2	GLU				83.759	33.159	22.625	1.00	20.00	8
	ATOM	2067	С	GLU	В	331		85.742	31.247	19.523	1.00	20.00	6
35	MOTA	2068	0	GLU	В	331		86.952	31.264	19.761	1.00	20.00	8
	ATOM	2069	N	GLY	В	332		85.257	31.137	18.292	1.00	20.00	7
	ATOM	2070	CA	GLY	В	332		86.145	31.159	17.140		20.00	6
	MOTA	2071	С	GLY	В	332		87.036	30.014	16.721	1.00	20.00	6
	ATOM	2072	0	GLY	В	332		86.881	28.863	17.142	1.00	20.00	8
40	ATOM	2073	N	TYR	В	333		88.002	30.366	15.875	1.00	20.00	7
	ATOM	2074	CA	TYR	В	333		88.939	29.413	15.307	1.00	20.00	6
	ATOM	2075	CB	TYR	В	333		89.625	30.053	14.093	1.00	20.00	6
	ATOM	2076	CG	TYR	В	333		88.724	30.031	12.877	1.00	20.00	6
	ATOM	2077	CD1	TYR	В	333		88.774	28.966	11.974	1.00	20.00	6
45	ATOM	2078	CE1	TYR	В	333		87.872	28.869	10.919		20.00	6
•	ATOM	2079		TYR				87.747	31.011	12.686		20.00	6
	MOTA	2080		TYR				86.831	30.923	11.624		20.00	6
	ATOM	2081	CZ	TYR				86.903	29.845	10.751		20.00	6
	ATOM	2082	OH	TYR				86.001	29.719	9.724		20.00	8
50	ATOM	2083	C	TYR				89.958	28.800	16.252		20.00	6
•	ATOM	2084	ō	TYR					27.721	15.971		20.00	8
	ATOM	2085	N	GLY				90.242	29.469	17.369		20.00	7
	ATOM	2086	CA	GLY				91.193	28.921	18.327		20.00	6
	ATOM	2087	CA	GLY				90.803	27.504	18.741		20.00	6
55	ATOM	2087							26.564			20.00	
"				GLY				91.577		18.558			8
	ATOM	2089	N	PRO				89.603	27.320	19.309		20.00	7
	ATOM	2090	CD	PRO				88.703	28.372	19.814		20.00	6
	ATOM	2091		PRO				89.145	25.991	19.731		20.00	6
	MOTA	2092	СВ	PRO	B	335		87.759	26.275	20.303	1.00	20.00	6

	ATOM	2093	CG	PRO	В 335	;	87.925	27.644	20.883	1.00 20.00	) 6
	ATOM	2094	Ċ	PRO	в 335		89.104	24.986			
	ATOM	2095	0		B 335		89.406	23.808	18.756	1.00 20.00	
	ATOM	2096	N		B 336		88.727	25.450	17.382		
5	ATOM	2097	CA		B 336		88.666			1.00 20.00	
,	ATOM	2098	CB					24.567	16.219	1.00 20.00	
					B 336		88.031	25.292	15.023	1.00 20.00	
	ATOM	2099	CG		В 336		88.051	24.581	13.663	1.00 20.00	
	ATOM	2100			B 336		87.486	23.177	13.787	1.00 20.00	6
	ATOM	2101			B 336		87.239	25.399	12.653	1.00 20.00	6
10	ATOM	2102	С		B 336		90.060	24.068	15.839	1.00 20.00	6
	ATOM	2103	0	LEU	B 336		90.274	22.870	15.665	1.00 20.00	
	ATOM	2104	N	LYS	в 337		91.011	24.986	15.717	1.00 20.00	
	ATOM	2105	CA	LYS	в 337		92.370	24.597	15.360	1.00 20.00	
	ATOM	2106	CB		в 337		93.198	25.848	15.046	1.00 20.00	
15	ATOM	2107	CG		B 337		92.678	26.560	13.801		
	ATOM	2108	CD		B 337		93.111	28.014		1.00 20.00	
	ATOM	2109	CE						13.717	1.00 20.00	
					B 337		94.561	28.167	13.314	1.00 20.00	
	ATOM	2110	NZ		В 337		94.882	29.611	13.122	1.00 20.00	
00	ATOM	2111	C		в 337		93.020	23.764	16.467	1.00 20.00	
20	ATOM	2112	0		в 337		93.965	23.015	16.215	1.00 20.00	8
	ATOM	2113	N		B 338		92.495	23.866	17.684	1.00 20.00	7
	ATOM	2114	CA	ALA	B 338		93.056	23.105	18.799	1.00 20.00	6
	MOTA	2115	CB	ALA	B 338		92.873	23.877	20.105	1.00 20.00	
	ATOM	2116	С	ALA	B 338		92.441	21.718	18.929	1.00 20.00	
25	ATOM	2117	0		в 338		92.805	20.955	19.820	1.00 20.00	8
	ATOM	2118	N		в 339		91.513	21.375	18.043	1.00 20.00	7
	ATOM	2119	CA		B 339		90.886	20.061	18.129	1.00 20.00	6
	ATOM	2120	СВ		B 339		89.786	19.919	17.074		
	ATOM	2121	CG		B 339		88.999	18.654		1.00 20.00	6
30	ATOM	2122			B 339		87.797		17.199	1.00 20.00	6
50	ATOM	2123						18.406	17.774	1.00 20.00	6
					B 339		89.462	17.440	16.737	1.00 20.00	7
	ATOM	2124			B 339		88.578	16.498	17.021	1.00 20.00	6
	ATOM	2125			B 339		87.559	17.057	17.650	1.00 20.00	7
2.5	ATOM	2126	C		в 339		91.928	18.952	17.970	1.00 20.00	6
35	ATOM	2127.			в 339	•	92.863	19.077	17.186	1.00 20.00	8
	MOTA	2128	N	PRO :	B 340		91.780	17.854	18.731	1.00 20.00	7
	ATOM	2129	CD	PRO 1	B 340		90.747	17.655	19.765	1.00 20.00	6
	ATOM	2130	CA	PRO 1	B 340		92.700	16.711	18.694	1.00 20.00	6
	MOTA	2131	CB	PRO 1	B 340		91.966	15.665	19.521	1.00 20.00	6
40	ATOM	2132	CG	PRO 1	B 340		91.310	16.505	20.579	1.00 20.00	6
	ATOM	2133	С	PRO I	B 340		93.072	16.198	17.301	1.00 20.00	6
	ATOM	2134	0	PRO I	B 340		94.193	15.748	17.080	1.00 20.00	8
	ATOM	2135	N	PHE I			92.139	16.270	16.362	1.00 20.00	7
	ATOM	2136	CA		B 341		92.407	15.797	15.011	1.00 20.00	6
45	MOTA	2137	СВ		B 341		91.152	15.943	14.142	1.00 20.00	_
	ATOM	2138	CG		B 341		91.317	15.424			6
	ATOM	2139		PHE I			91.517		12.738	1.00 20.00	6
	ATOM	2140		PHE I				14.080	12.507	1.00 20.00	6
							91.182	16.277	11.647	1.00 20.00	6
50		.2141		PHE E			91.738	13.592	11.207	1.00 20.00	6
50	ATOM	2142		PHE E			91.320	15.803	10.345	1.00 20.00	6
	ATOM	2143	CZ	PHE E			91.599	14.457	10.123	1.00 20.00	6
	ATOM	2144		PHE E			93.571	16.550	14.362	1.00 20.00	6
	ATOM	2145		PHE E			94.268	16.002	13.514.	1.00 20.00	8
	ATOM	2146	N	PHE E	3 3 4 2		93.777	17.800	14.765	1.00 20.00	7
55	ATOM	2147	CA	PHE E	3 3 4 2		94.842	18.630	14.202	1.00 20.00	6
	ATOM	2148	CB	PHE · E	3 342		94.336	20.058	13.975	1.00 20.00	6
	ATOM	2149	CG	PHE E	342		93.124	20.152	13.096	1.00 20.00	6
	ATOM	2150		PHE E			93.166	19.729	11.777	1.00 20.00	6
	ATOM	2151		PHE E			91.954	20.734	13.575	1.00 20.00	6
										2.00 20.00	v

5	ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2152 2153 2154 2155 2156 2157 2158		PHE PHE GLU GLU	B B B B	342 342 342 342 343 343		92.058 90.843 90.898 96.077 96.932 96.173 97.293	19.8 20.8 20.4 18.7 19.5 17.8 17.8	98 12.742 75 11.423 18 15.101 84 14.902 29 16.083	2 1.00 3 1.00 1 1.00 2 1.00 3 1.00	20.00 20.00 20.00 20.00 20.00 20.00 20.00	6 6 6 8 7 6
10	ATOM ATOM ATOM ATOM	2159 2160 2161 2162 2163	OE2	GLU GLU GLU	B B B	343		97.330 98.475 98.372 98.290 98.379	16.50 16.53 15.30 14.20 15.62	25 18.839 65 19.813 01 19.359 22 21.036	1.00 3 1.00 9 1.00 5 1.00	20.00 20.00 20.00 20.00 20.00	6 6 8 8
15	ATOM ATOM ATOM ATOM ATOM ATOM	2164 2165 2166 2167 2168 2169	C O N CA CB OG	GLU SER SER SER	B B B	343 344 344 344 344	1	98.683 99.419 99.047 100.370 100.848 100.072	18.13 18.90 17.38 17.54 16.23	59 16.925 32 15.383 19 14.781 19 14.192	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00 20.00	6 8 7 6 6 8
20	ATOM ATOM ATOM ATOM ATOM	2170 2171 2172 2173 2174	C O N CA CB	SER SER VAL VAL	B B B	344 344 345	3	100.467 101.485 99.423 99.430 97.985	18.62 18.73 19.43 20.48	29 13.702 32 13.025 35 13.544 36 12.527	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	6 8 7 6
25	MOTA MOTA MOTA MOTA MOTA	2175 2176 2177 2178 2179		VAL VAL VAL VAL THR	B B B	345 345 345		98.015 97.335 00.096 99.844 00.951	22.04 19.64 21.78 22.27 22.33	12 11.120 16 11.400 35 12.980 75 14.085	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	6 6
30	MOTA MOTA MOTA MOTA	2180 2181 2182 2183 2184		THR THR THR THR	B B	346 346 346	· 1 1 1	.01.602 .03.096 .03.816 .03.707	23.61 23.59 22.68 24.98 24.57	93 11.982 88 12.831 83 12.115	1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	6 8 6 6
35	MOTA MOTA MOTA MOTA MOTA	2185 2186 2187 2188 2189	O N CA CB CG	THR TRP TRP TRP	B B B	347 347 347 347	1	.00.950 99.966 99.089 97.941 97.088	24.56 25.38 26.30 26.72 25.59	35 12.138 36 11.425 37 12.344 34 12.818	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	8 7 6 6 6
40	ATOM ATOM ATOM ATOM ATOM	2190 2191 2192 2193 2194	CE2 CE3 CD1	TRP TRP TRP TRP	B B B	347 347 347		95.924 95.436 95.247 97.259 96.269	25.07 24.00 25.39 24.84 23.89	12.963 7 10.983 8 13.953	1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	6 6 6 7
45	ATOM ATOM ATOM ATOM ATOM	2195 2196 2197 2198 2199	CZ3	TRP TRP TRP	B B B	347 347 347 347	· · ·	94.300 94.113 93.654 99.679 99.101	23.61 27.56 28.11	1 10.636 0 11.452 3 10.800 4 9.867	1.00 1.00 1.00 1.00	20.00 20.00 20.00	6 6 6 8
50	ATOM ATOM ATOM ATOM ATOM	2200 2201 2202 2203 2204	N CA CB C	ALA ALA ALA ALA ALA	В В В	348 348 348 348	1 1 1	00.820 01.439 02.582 01.933 01.874	28.01 29.24 29.65 29.27 30.32	7 10.822 6 11.761 7 9.381 3 8.738	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00	7 6 6 6 8
55	ATOM ATOM ATOM ATOM ATOM ATOM	2205 2206 2207 2208 2209 2210		ASN ASN ASN ASN ASN	B B B	349 349 349 349	1 1 1	02.411 02.940 04.466 05.058 04.445 06.251	28.15 28.20 26.92 26.28 26.56	3 7.500 5 7.569 9 8.138 2 8.984	1.00 1.00 1.00 1.00	20.00 20.00 20.00 20.00 20.00 20.00	7 6 6 8 7

							100 500	06.066	c co.	1 00		_
	ATOM	2211	С	ASN			102.522	26.966	6.634		20.00	6
	ATOM	2212	0	ASN			103.353	26.371	5.944		20.00	8
	ATOM	2213	N	LEU			101.242	26.628	6.643		20.00	7
	ATOM	2214	CA	LEU		350	100.776	25.500	5.846		20.00	
5	MOTA	2215	СВ	LEU		350	99.257	25.355	5.973		20.00	6
	MOTA	2216	CG	LEU		350	98.734	24.848	7.316		20.00	6
-	ATOM	2217		LEU		350	97.244	25.127	7.418		20.00	6
	ATOM	2218	CD2	LEU	В	350	99.030	23.357	7.444		20.00	6
	ATOM	2219	С	LEU	В	350	101.147	25.574	4.365		20.00	6
10	ATOM	2220	0	LEU	В	350	101.557	24.575	3.775		20.00	8
	ATOM	2221	N	HIS	В	351	101.006	26.744	3.752	1.00	20.00	7
	ATOM	2222	CA	HIS	В	351	101.305	26.829	2.329	1.00	20.00	6
	ATOM	2223	СВ	HIS	В	351	100.651	28.087	1.721	1.00	20.00	6
	ATOM	2224	CG	HIS	В	351	101.553	29.274	1.618	1.00	20.00	6
15	ATOM	2225		HIS		351	102.001	30.143	2.556	1.00	20.00	6
	ATOM	2226		HIS			102.072	29.706	0.416	1.00	20.00	7
	MOTA	2227		HIS		351	102.798	30.792	0.618	1.00	20.00	6
	ATOM	2228	NE2			351	102.772	31.079	1.907	1.00	20.00	7
	ATOM	2229	C	HIS			102.797	26.731	1.999	1.00	20.00	6
20	ATOM	2230	Ö	HIS		351	103.176	26.669	0.832		20.00	8
20	ATOM	2231	Ŋ	GLN			103.634	26.685	3.033		20.00	7
	MOTA	2232	CA			352	105.081	26.554	2.851		20.00	6
	ATOM	2233	CB	GLN		352	105.841	27.458	3.819		20.00	6
		2234	CG			352		28.705	3.166		20.00	6
25	ATOM		CD			352	105.930		3.854		20.00	6
25	ATOM	2235			-	352·	106.134	30.139	5.053		20.00	8
	ATOM	2236	OE1				105.299	30.854	3.096		20.00	7
	ATOM	2237	NE2			·352 352	105.299	25.099	3.088		20.00	6
	ATOM	2238	C			352.	106.632	24.715	2.895		20:00	8
20	ATOM	2239	0				104.514	24.715	3.522		20.00	7
30	ATOM	2240	N			353	•	22.888	3.777		20.00	6
	ATOM	2241	CA	GLN		353	104.761	22.395	4.900		20.00	6
	ATOM	2242	CB	GLN		353	103.849	23.050	6.240		20.00	6
	ATOM	2243	CG			353	104.122	22.711	7.281		20.00	6
	ATOM	2244	CD	GLN		353	103.075	21.571	7.201		20.00	8
35	MOTA	2245	OE1			353	102.627		8.076		20.00	7
	ATOM	2246	NE2			353	102.690	23.700	2.510		20.00	6
	ATOM	2247	C	GLN		353	104.507	22.079 22.490	1.641		20.00	8
	ATOM	2248	0	GLN		353	103.732		2.401		20.00	7
	MOTA	2249	N	THR		354	105.172	20.937	1.244		20.00	6
40	MOTA	2250	CA	THR		354	104.998	20.071	1.029		20.00	6
•	MOTA	2251	СВ	THR		354	106.240	19.173	0.790		20.00	8
	ATOM	2252	OG1	THR		354	107.390	19.999			20.00	6
	ATOM	2253	CG2	THR		354	106.033	18.243	-0.166		20.00	6
	MOTA	2254	C			354	103.777	19.197	1.501			8
45	MOTA	2255	0			354	103.745	18.426	2.454		20.00	
	MOTA	2256	N			355	102.741	19.319	0.658			7
	MOTA	2257	CD			355	102.547	20.275	-0.444		20.00	6
	MOTA	2258	CA			355	101.540	18.505	0.859		20.00	6
	ATOM	2259	СВ			355	100.616	18.967	-0.266		20.00	6
50	MOTA	2260	CG			355	101.039	20.387	-0.490		20.00	6
	MOTA	2261	C			355	101.835	17.011	0.766		20.00	
	ATOM	2262	O.			355	102.631	16.577	-0.065		20.00	8
	MOTA	2263	N			356	101.198	16.204	1.625		20.00	7
	MOTA	2264	CD			356	100.128	16.522	2.587		20.00	6
55	MOTA	2265	CA			356	101.438	14.761	1.573		20.00	6
	ATOM	2266	CB			356	100.593	14.235	2.729		20.00	6
	ATOM	2267	CG			356	99.429	15.188	2.737		20.00	6
	MOTA	2268	С			356	100.960	14.244	0.222		20.00	6
	ATOM	2269	0	PRO	В	356	100.005	14.779	-0.346	1.00	20.00	8

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ATOM
             2270
                   N
                        ALA B 357
                                       101.629
                                                 13.221
                                                         -0.300
                                                                  1.00 20.00
                                                         -1.588
      ATOM
             2271
                   CA
                        ALA B 357
                                       101.247
                                                 12.660
                                                                  1.00 20.00 6
      MOTA
             2272
                   CB
                        ALA B 357
                                       102.352
                                                 11.750
                                                         -2.118
                                                                  1.00 20.00 6
      ATOM
             2273
                   С
                        ALA B 357
                                        99.948
                                                 11.883
                                                         -1.427
                                                                  1.00 20.00
      ATOM
             2274
                                        99.808
                                                11.074
                                                         -0.506
                   0
                        ALA B 357
                                                                  1.00 20.00
     ATOM
             2275
                        LEU B 358
                                        99.000
                   N
                                                12.134
                                                         -2.323
                                                                  1.00 20.00
                                                                              7
     ATOM
             2276
                   CA
                       LEU B 358
                                        97.709
                                                11.460
                                                         -2.278
                                                                  1.00 20.00
                                                                               6
     ATOM
             2277
                   CB
                        LEU B 358
                                        96.729
                                                 12.166
                                                         -3.217
                                                                  1.00 20.00
                                                                               6
     ATOM
             2278
                   CG
                        LEU B 358
                                        96.368
                                                 13.582
                                                         -2.766
                                                                  1.00 20.00
                                                                               6
10
                   CD1 LEU B 358
             2279
                                        95.513
                                                         -3.813
     ATOM
                                                 14.262.
                                                                  1.00 20.00
                                                                               6
     MOTA
             2280
                   CD2 LEU B 358
                                        95.636
                                                 13.516
                                                         -1.430
                                                                  1.00 20.00
                                                                               6
             2281
                        LEU B 358
                                        97.813
                                                 9.976
                                                         -2.633
     ATOM
                   C
                                                                  1.00 20.00
                                                                               6
     ATOM
             2282
                   0
                        LEU B 358
                                        97.918
                                                 9.614
                                                         -3.806
                                                                  1.00 20.00
                                                                               8
     ATOM
             2283
                        THR B 359
                                        97.776
                                                 9.134
                                                         -1.600
                   N
                                                                  1.00 20.00
                                                                               7
15
     MOTA
             2284
                   CA
                       THR B 359
                                        97.867
                                                 7.678
                                                         -1.735
                                                                  1.00 20.00
             2285
     MOTA
                   CB
                       THR B 359
                                        96.513
                                                 7.046
                                                         -2.149
                                                                  1.00 20.00
     ATOM
             2286
                   OG1 THR B 359
                                        96.111
                                                 7.555
                                                         -3.427
                                                                  1.00 20.00
                                                                              8
     ATOM
             2287
                   CG2 THR B 359
                                        95.439
                                                 7.355
                                                         -1.112
                                                                  1.00 20.00
                                                                               6
     ATOM
             2288
                   С
                        THR B 359
                                        98.933
                                                 7.238
                                                         -2.736
                                                                  1.00 20.00
                                                                               6
20
     MOTA
             2289
                   0
                        THR B 359
                                        99.903
                                                 7.998
                                                         -2.945
                                                                  1.00 20.00
                                                                             . 8
             2290
     MOTA
                   OXT THR B 359
                                        98.802
                                                  6.121
                                                         -3.280
                                                                  1.00 20.00 8
     TER
     MOTA
             2291
                   OH2 TIP S
                                        42.566
                                                19.118
                                                         34.302
                                                                  1.00 15.09
                                1
     MOTA
             2292
                   OH2 TIP S
                                2
                                        41.052
                                                32.378
                                                        19.857
                                                                  1.00 15.82
25
     MOTA
             2293
                   OH2 TIP S
                                3
                                        37.014
                                                33.030
                                                        17.747
                                                                  1.00 16.95
     MOTA
             2294
                   OH2 TIP S
                                        45.353
                                                24.370
                                                        18.152
                                5
                                                                  1.00 16.85
                                                                  1.00 20.42
     ATOM
             2295
                   OH2 TIP S
                                6
                                        31.896
                                                13.930
                                                         33.235
                                                                                   S
     ATOM
             2296
                   OH2 TIP S
                                7
                                        50.351
                                                22.781
                                                         28.249
                                                                  1.00 21.14
                                                                                   s
                               . 8
     ATOM
             2297
                   OH2 TIP S
                                        45.246
                                                -0.589
                                                         -0.734
                                                                  1.00 17.74
                                                                                   S
                                                         -8.523
30
             2298
                   OH2 TIP S
                                        46.249
                                                -0.348
                                                                  1.00 21.32
     ATOM
                               11
                                                                                   S
                   OH2 TIP S
                                                                  1.00 21.94
             2299
                                        45.756
                                                         29.680
     MOTA
                               14
                                                11.148
                                                                                   S
     MOTA
             2300
                   OH2 TIP S
                               15
                                        44.273
                                                13.157
                                                         34.592
                                                                  1.00 15.61
                                                                                   s
     MOTA
             2301
                   OH2 TIP S
                               17
                                        53.598
                                                 3.722
                                                         -1.720
                                                                  1.00 21.45
                                                         31.565
                                        46.049
                                                                  1.00 20.35
     MOTA
             2302
                   OH2 TIP S
                               18
                                                13.087
.35
     MOTA
             2303
                   OH2 TIP S
                               19
                                        53.422
                                                22.401
                                                         -3.280
                                                                 1.00 23.26
                                                                                   S
     ATOM
             2304
                   OH2 TIP S
                               20
                                        34.587
                                                 7.922
                                                          5.383
                                                                 1.00 22.58
                                                                                   S
     ATOM
             2305
                       TIP S
                                        45.053
                                                27.379
                                                         19.376
                                                                 1.00 29.60
                   OH2
                               21
                                                                                   S
     ATOM
             2306
                   OH2 TIP S
                               23
                                        28.899
                                                36.416
                                                         28.633
                                                                  1.00.31.68
                                                                                   s
            .2307
     MOTA
                   OH2 TIP S
                                        35.531
                                                11.645
                                                         -8.219
                                                                 1.00 23.45
                               24
                                                                                   S
40
             2308
                   OH2 TIP S
                                        47.364
                                                28.787
                                                         19.612
                                                                 1.00 23.03
     MOTA
                               25
                                                                                   S
     MOTA
             2309
                   OH2 TIP S
                               27
                                       48.859
                                                21.588
                                                        12.634
                                                                 1.00 23.76
     ATOM
             2310
                   OH2 TIP S
                               29
                                       48.805
                                                 8.920
                                                        23.626
                                                                 1.00 22.23
                   OH2 TIP S
                                        48.619
     ATOM
             2311
                               31-
                                                 7.247
                                                         10.112
                                                                 1.00 21.32
                                                                                   S
                   OH2 TIP S
     ATOM
             2312
                               34
                                        44.824
                                                28.720
                                                        15.621
                                                                 1.00 25.27
                                                                                  S
     ATOM
             2313
                   OH2 TIP S
                               35
                                        26.030
                                                12.634
                                                         13.407
                                                                 1.00 21.61
                                                                                  S
     ATOM
             2314
                   OH2 TIP S
                               36
                                        50.462
                                                19.810
                                                         40.066
                                                                 1.00 25.45
                                                                                   S
     ATOM
             2315
                   OH2 TIP S
                               37
                                       39.631
                                                23.510
                                                         -0.239
                                                                 1.00 30.88
                                                                                  S
                                       44.734
     ATOM
             2316
                   OH2 TIP S
                                                42.655
                                                         10.346
                                                                 1.00 30.84
                               40
                                                                                  S
                                       54.653
                                                3.902
                                                                 1.00 27.14
     ATOM
             2317
                   OH2 TIP S
                               41
                                                         1.503
                                                                                  S
50
     ATOM
             2318
                   OH2 TIP S
                               45
                                       45.693
                                                21.923
                                                         39.754
                                                                 1.00 28.30
                                                                                  S
     MOTA
             2319
                   OH2 TIP S
                               47
                                        47.820
                                                16.413
                                                          7.805
                                                                 1.00 25.73
                                       50.292
     ATOM
             2320
                   OH2 TIP S
                               48
                                                31.412
                                                         29.642
                                                                 1.00 32.79
     MOTA
             2321
                   OH2 TIP S
                               49
                                       26.056
                                                16.646
                                                         34.827
                                                                 1.00 29.80
                                                                                  S
     ATOM
             2322
                   OH2 TIP S
                               52
                                       31.714
                                                10.996
                                                         31.855
                                                                 1.00 29.15
                                                                                  S
     ATOM
             2323
                       TIP S
                               53
                                       46.108
                                                23.843
                                                                 1.00 24.21
                   OH2
                                                         -4.299
     ATOM
             2324
                   OH2
                       TIP S
                               54
                                       37.645
                                                11.206
                                                         34.448
                                                                 1.00 28.56
                                                                                  s
                   OH2 TIP S
     ATOM
             2325
                               55
                                       26.371
                                                28.513
                                                        12.142
                                                                 1.00 32.08
                                                                                  S
                   OH2 TIP S
                               58
                                       33.564
     MOTA
             2326
                                                19.700
                                                         3.483
                                                                 1.00 28.28
                                                                                  S
                                       48.295
     MOTA
             2327
                   OH2 TIP S
                              64
                                                -0.632
                                                        14.280
                                                                 1.00 32.13
```

	ATOM .	2328	OH2 TIP S	65	40.064	26.036	34.324	1.00 24.17	s
	ATOM	2329	OH2 TIP S	66	29.570	3.958	14.729	1.00 28.94	S
	MOTA	2330	OH2 TIP S	72	60.085	11.604	6.814	1.00 38.35	S
	MOTA	2331	OH2 TIP S	73	39.203	44.403	18.686	1.00 26.61	S
5	MOTA	2332	OH2 TIP S	76	47.312	12.366	27.366	1.00 28.51	S
	MOTA	2333	OH2 TIP S	8.0	43.862	33.771	33.329	1.00 28.82	S
	ATOM	2334	OH2 TIP S	81	57.890	13.106	2.128	1.00 40.62	S
	MOTA	2335	OH2 TIP S	82	41.663	34.381	32.043	1.00 19.35	S
	ATOM	2336	OH2 TIP S	85	50.974	40.331	19.200	1.00 21.14	S
10	ATOM	2337	OH2 TIP S	88	47.925	-0.832	-6.556	1.00 24.11	S
	MOTA	2338	OH2 TIP S	90	27.231	28.336	33.481	1.00 27.64	S
	MOTA	2339	OH2 TIP S	91	43.651	-7.101	-7.995	1.00 24.33	S
	MOTA	2340	OH2 TIP S	92	49.325	4.387	19.370	1.00 28.02	S
	MOTA	2341	OH2 TIP S	93	46.231	11.549	33.898	1.00 29.40	S
15	MOTA	2342	OH2 TIP S	94	63.889	24.831	1.168	1.00 26.53	S
	ATOM	2343	OH2 TIP S	96	56.396	4.952	-6.749	1.00 28.00	s
	MOTA	2344	OH2 TIP S	98	35.510	27.986	11.558	1.00 29.24	Ś
	ATOM	2345	OH2 TIP S	100	49.942	24.366	30.265	1.00 31.61	S
	ATOM	2346	OH2 TIP S	101.	56.121	7.113	-8.298	1.00 31.57	S
20	ATOM ·	2347	OH2 TIP S		58.318	19.957	-8.378	1.00 26.95	S
	MOTA	2348	OH2 TIP S		49.647	22.446	39.624	1.00 40.57	S
	ATOM	2349	OH2 TIP S		45.359	7.052	13.052	1.00 26.27	S
	ATOM	2350	OH2 TIP S		37.150	32.340	32.346	1.00 34.45	S
	ATOM	2351	OH2 TIP S		43.465	40.457	8.240	1.00 40.48	S
25	MOTA	2352	OH2 TIP S		36.644	8.257	13.418	1.00 30.70	S
	ATOM	2353	OH2 TIP S		41.912	-8.974	-8.264	1.00 26.08	S
	ATOM	2354		124	62.424	15.800	-7.411	1.00 24.08	S
	ATOM	2355	OH2 TIP S		37.266	18.656	-9.097	1.00 28.99	S
	MOTA	2356			43.129	26.845	14.606	1.00 25.19	S
30	ATOM	2357	OH2 TIP S		36.339	32.639	29.802	1.00 29.25	S
	ATOM	2358	OH2 TIP S		54.051	14.561	26.498	1.00 33.93	S
	ATOM	2359	OH2 TIP S		41.805	-4.242	5.492	1.00 33.72	· s
	ATOM	2360	OH2 TIP S		38.873	25.163	36.697	1.00 30.69	S
26	ATOM	2361.	OH2 TIP S		28.777	8.553	25.307	1.00 31.43	s
35	ATOM	2362	OH2 TIP S		53.672		-12.803	1.00 33.45	S
	ATOM	2363	OH2 TIP S		59.892	15.434	11.467	1.00 31.39	S
	ATOM	2364	OH2 TIP S		31.040	12.361	35.470	1.00 34.07	s
	ATOM	2365			33.489 46.918	14.292	-0.598	1.00 40.68	S
40	ATOM ATOM	2366 2367			46.297	8.748	11.662 -9.196	1.00 29.23	S S
40	ATOM	2368	OH2 TIP S		58.193	-7.287 6.715		1.00 42.20	S
	ATOM	2369			44.598	4.435	-4.685 12.503	1.00 35.48 1.00 27.68	S
	ATOM	2370	OH2 TIP S		27.003	5.999	12.450	1.00 27.00	S
	ATOM	2371	OH2 TIP S		43.676	32.852	35.735	1.00 35.70	S
45	ATOM	2372						1.00 34.62	S
7.5	ATOM	2373	OH2 TIP S			4.058	20.638	1.00 34.02	S
	ATOM	2374	OH2 TIP S		45.839	35.853	33.724	1.00 45.03	S
		2375	OH2 TIP S		22.176	18.976	16.752	1.00 33.47	s
	ATOM	. 2376	OH2 TIP S		43.986	33.179	10.162	1.00 31.07	s
50	ATOM	2377	OH2 TIP S		50.653	20.347	42.428	1.00 35.80	s
	ATOM	2378	OH2 TIP S		47.843	24.314	9.506	1.00 31.05	S
	ATOM	2379	OH2 TIP S		44.693		-14.175	1.00 29.90	S
	ATOM	2380	OH2 TIP S		26.560	36.851	31.684	1.00 49.29	S
	ATOM	2381	OH2 TIP S				-12.951	1.00 49.25	S
55	ATOM	2382	OH2 TIP S		30.432	28.741	12.438	1.00 23.21	S
	ATOM	2383	OH2 TIP S		41.004	20.553	6.423	1.00 37.70	S
	ATOM	2384	OH2 TIP S		49.258	20.069	29.294	1.00 33.97	S
	ATOM	2385	OH2 TIP S		48.082	28.459	16.489	1.00 33.10	S
	ATOM	2386	OH2 TIP S		47.448	18.625	27.683	1.00 34.87	S
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	ATOM ATOM	2387 2388	OH2 TIP S		19.687 32.402	20.632 -1.266	23.411 22.443	1.00 35.01 1.00 37.26	s s
	ATOM	2389	OH2 TIP S		39.475	33.468	33.237	1.00 37.20	S
	ATOM	2390	OH2 TIP S		44.277	18.950	5.162	1.00 35.34	S
5	ATOM	2391	OH2 TIP S		34.797	30.523	10.736	1.00 47.55	S
,	MOTA	2392	OH2 TIP S				-14.949	1.00 47.55	S
	ATOM	2393	OH2 TIP S		36.333	16.371	1.539	1.00 28.54	S
	ATOM	2394	OH2 TIP S		46.761	38.936	27.403	1.00 34.66	S
	ATOM	2395	OH2 TIP S		24.163	13.264	11.375	1.00 34.00	S
10	ATOM	2396	OH2 TIP S		48.459	15.018	31.951	1.00 38.11	S
10	ATOM	2397	OH2 TIP S		34.261	23.193	40.004	1.00 48.96	S
	ATOM	2398	OH2 TIP S		45.924	-0.026	13.224	1.00 40.50	
	ATOM	2399	OH2 TIP S		41.384	37.389	32.543	1.00 40.74	. S
	ATOM	2400	OH2 TIP S		49.394	35.312	27.150	1.00 44.33	s
15	ATOM	2400	OH2 TIP S		29.066	29.942	34.359	1.00 41.46	S
.13	ATOM	2402	OH2 TIP S		49.354	19.467	7.273	1.00 34.56	S
	ATOM	2403	OH2 TIP S		25.298	17.029	31.863	1.00 47.74	S
	ATOM	2404	OH2 TIP S		37.071	25.027	4.669	1.00 47.74	S
	ATOM	2405	OH2 TIP S		22.581	7.487	18.691	1.00 41.75	S
20	ATOM	2406	OH2 TIP S		32.269	7.011	-1.891	1.00 41.73	S
20	ATOM	2407	OH2 TIP S		48.234	0.494	6.833	1.00 48.16	S
	ATOM	2408	OH2 TIP S		20.008	14.658	19.211	1.00 45.27	S
	ATOM	2409	OH2 TIP S		49.341	22.698	42.272	1.00 42.20	s
	ATOM	2410	OH2 TIP S		61.292	18.260	-8.097	1.00 45.21	S
25	ATOM	2411	OH2 TIP S		28.152	10.606	2.819		· s
23	ATOM	2412	OH2 TIP S		25.626	12.619	23.191	1.00 34.27	S
	ATOM	2413	OH2 TIP S		59.876	11.603	1.216	1.00 46.54	S
	ATOM	2414	OH2 TIP S		57.592		-10.646	1.00 45.82	S
	ATOM	2415	OH2 TIP S		31.509	36.649	21.499	1.00 38.73	s
30	ATOM	2416	OH2 TIP S		50.270	-1.543	-6.136	1.00 42.66	S
	ATOM	2417	OH2 TIP S		24.467	8.729	13.088	1.00 42.78	s
	ATOM	2418	OH2 TIP S		38.098	8.699	25.759	1.00 32.80	S
	ATOM	2419	OH2 TIP S		57.831		-13.255	1.00 45.31	s
	ATOM	2420	OH2 TIP S		23.888	22.328	30.524	1.00 37.12	
35	ATOM	2421	OH2 TIP S	202	47.691	26.068	37.666	1.00 37.92	s
	ATOM	2422	OH2 TIP S	203	38.653	7.070	29.307	1.00 50.54	s
	MOTA	2423	OH2 TIP S	206	44.424	27.583	2.092	1.00 53.50	s
	MOTA	2424	OH2 TIP S	212	22.258	2.296	17.948	1.00 47.38	S
	MOTA	2425	OH2 TIP S	214	19.843	17.943	23.303	1.00 30.36	s
40	MOTA	2426	OH2 TIP S	216	27.647	11.344	24.681	1.00 31.32	S
	ATOM	2427	OH2 TIP S	217	37.953	7.817	-9.284	1.00 45.97	S
	MOTA	2428	OH2 TIP S	218	33.845	34.040	12.124	1.00 38.11	S
	ATOM	2429	OH2 TIP S		58.484	15.269	13.717	1.00 38.26	
	ATOM	2430	OH2 TIP S		48.526	40.920	26.583	1.00 35.23	S
45	ATOM	2431	OH2 TIP S	222	52.094	21.184		1.00 29.86	s
	ATOM	2432	OH2 TIP S		36.889	5.881	3.281	1.00 37.63	S
	MOTA	2433	OH2 TIP S				-10.684	1.00 34.89	S
	MOTA	2434	OH2 TIP S		47.284	2.916	19.133	1.00 34.10	S
	ATOM	2435	OH2 TIP S		42.468		-15.039	1.00 37.98	S
50	MOTA	2436	OH2 TIP S		19.169	22.832	21.831	1.00 41.57	S
	MOTA	2437	OH2 TIP S		57.592	12.689	14.880	1.00 50.22	. S
	MOTA	2438	OH2 TIP S		27.102	9.176	5.655	1.00 40.57	s
	ATOM	2439	OH2 TIP S			9.072		1.00 50.71	S
	ATOM	2440	OH2 TIP S		22.822	25.342	19.945	1.00 34.93	S
55	ATOM	2441	OH2 TIP S		24.831	32.218	28.901	1.00 37.69	S
	ATOM	2442	OH2 TIP S		20.045	10.774	16.992	1.00 39.57	S
	ATOM	2443	OH2 TIP S		58.019	19.850	15.679	1.00 41.42	S
	ATOM	2444	OH2 TIP S		19.490	20.949	26.114	1.00 34.55	S
	ATOM	2445	OH2 TIP S	240	61.187	26.377	7.346	1.00 39.68	Ş

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	ATOM	2446	OH2 TIP	S 241		33.680	38.342	19.389	1.00	48.93	s
	ATOM	2447	OH2 TIP			51.539	31.612			55.65	S
	MOTA	2448	OH2 TIP			25.872	14.431			46.69	S
	ATOM	2449	OH2 TIP			37.332					
-							5.849			43.81	S
5	MOTA	2450	OH2 TIP		•	39.087	-1.293			42.96	S
	ATOM	2451		S 258		23.938	30.000			38.89	s
	MOTA	2452		S 259		24.949	29.749	32.578	1.00	40.17	s
	MOTA	2453	OH2 TIP	S 260		32.111	17.986	1.918	1.00	48.36	S
	MOTA	2454	OH2 TIP	S 266		21.404		25,603	1.00	57.17	· s
10	ATOM	2455	OH2 TIP	S 269		35.425	36.767			30.70	S
	ATOM	2456	OH2 TIP			52.438	25.529			44.85	s
	ATOM	2457	OH2 TIP			53.299	20.156			37.15	S
	ATOM	2458		S 272							
						50.914	6.919			43.29	S
	ATOM	2459	OH2 TIP			31.578	30.795	11.014		50.15	S
15	MOTA	2460		S 275		26.341	7.243	22.447		39.40	S
	ATOM	2461		S 276		60.392	18.195	10.235	1.00	37.91	s
	ATOM	2462	OH2 TIP	S 277		47.355	-9.081	-10.821	1.00	48.18	S
	ATOM	2463	OH2 TIP	S 279		41.304	6.175	-16.647	1.00	38.12	S
	ATOM	2464	OH2 TIP	S 282		33.299	21.620		1.00	46.29	S
20	ATOM	2465	OH2 TIP			56.469	26.112	-8.575		43.71	S
20	ATOM	2466	OH2 TIP			48.382	26.573	7.246		41.43	s
	ATOM	2467	OH2 TIP			56.240		-11.331		41.79	
			OH2 TIP								S
	ATOM	2468				49.060	14.978	28.166		37.03	S
	ATOM	2469	OH2 TIP			37.095	44.270	26.442		45.08	S
25	MOTA	2470	OH2 TIP			47.814		-13.299		48.60	S
•	MOTA	2471	OH2 TIP	S 297		58.081	2.784	-7.841	1.00	41.89	S
	ATOM	2472	OH2 TIP	S 298		36.447	45.321	18.644	1.00	54.91	S
	ATOM	2473	OH2 TIP	S 299		49.029	23.328	1.767	1.00	30.55	S
	ATOM	2474	OH2 TIP	S 301		24.375	13.771	8.634	1.00	48.47	S
30	ATOM	2475	OH2 TIP	S 303		47.904	36.798	28.653		35.76	s
	ATOM	2476	OH2 TIP			51.156	40.821	27.172		43.59	S
	ATOM	2477	OH2 TIP			32.943	28.917	35.227		42.60	S
	ATOM	2478		S 307		58.462	28.373	6.251		46.15	S
25	ATOM	2479		s 308		41.964	30.940	36.712		48.26	S
35	ATOM	2480		S 313		51.176	-1.922	-3.336		50.61	S
	MOTA	2481		S1001		21.319	36.868	23.805		36.97	S
	ATOM	2482	OH2 TIP			48.880	32.620	27.617	1.00	44.40	S
	ATOM	2483	OH2 TIP	S1003		61.880	19.473	11.767	1.00	45.49	S
	ATOM	2484	OH2 TIP	S1004		52.770	21.424	26.815	1.00	24.43	s
40	ATOM	2485	OH2 TIP	S1005		35.373	29.094	36.197	1.00	35.97	s
	ATOM	2486	OH2 TIP			40.815	-6.636	4.389	1.00	43.15	s
	ATOM	2487	OH2 TIP			44.953	1.286	11.272	1.00	49.45	S
	ATOM	2488	OH2 TIP			21.004	16.168	27.009		48.51	s
	ATOM	2489	OH2 TIP			47.094	41.786	9.243		50.10	S
45	ATOM	2490									_
45			OH2 TIP			32.479	2.978			49.47	S
	ATOM	2491	012 GLC			48.557		-12.279		40.72	G
	ATOM	2492	C11 GLC			48.836		-11.097		38.05	G
	ATOM	2493	C13 GLC			49.266		-11.476		38.09	G
	ATOM	2494	O14 GLC	G .1		49.559	14.299	-10.292	1.00	33.99	G
50	ATOM	2495	C15 GLC	G 1		48.150	14.257	-12.257	1.00	37.32	G
	ATOM	2496	016 GLC	G 1		48.574	15.582	-12.604	1.00	36.74	G
	ATOM	2497	012 GLC	G 2		40.114	-6.634	-6.562		33.52	G
	ATOM	2498	C11 GLC			38.967	-6.592	-7.404		31.05	Ğ
	ATOM	2499	C13 GLC			37.712	-6.417	-6.552		31.56	G
55	ATOM	2500	O14 GLC			36.554	-6.406	-7.389		30.70	G
55	ATOM	2501									
			C15 GLC			37.792	-5.109	-5.761		30.03	G
	ATOM	2502	016 GLC			36.609	-4.961	-4.975		29.66	G
	ATOM	2503	012 GLC			44.030		-13.470		37.90	G
	MOTA	2504	C11 GLC	G 3		43.950	9.648	-13.690	1.00	38.47	G

	ATOM	2505	C1	3 GL	C G	3	42.747	9.974	-14.579	1.00 39.52	~
	ATOM	2506		4 GL			41.551	9 526	-13.942	1.00 39.32	G
	ATOM	2507		5 GL		3	42.878	9 280	-15.934		G
	ATOM	2508		6 GL						1.00 41.43	G
5						3	41.736		-16.731	1.00 40.78	G
,	ATOM	2509		2 GL		5.	40.556	1.005	2.289	1.00 45.25	G
	ATOM	2510		1 GL		5	40.966	2.332	1.960	1.00 40.56	G
	ATOM	2511		3 GL(		5	40.187	3.327	2.814	1.00 40.36	G
	MOTA	2512	014	4 GLO	G	5	38.791	3.169	2.572	1.00 40.71	G
	ATOM	2513	C1!	5 GLO	G	5	40.619	4.751	2.464	1.00 40.04	G
10	ATOM	2514	016	6 GLO	G	5	39.885	5.681	3.256	1.00 36.89	G
	ATOM	2515	012	2 GLC	G	6	36.951	22.702	40.046	1.00 63.04	G
	ATOM	2516	C11	l GLC	. G	6	37.592	21.583	39.422	1.00 62.46	G
	ATOM	2517		3 GLC	_	6	38.104	21.978	38.030	1.00 61.14	
	ATOM	2518		4 GLC		6	39.034	23.054			G
15	ATOM	2519		5 GLC	-	6			38.168	1.00 61.72	G
13	ATOM						36.948	22.429	37.126	1.00 60.51	G
		2520		GLC		6	35.992	21.372	36.960	1.00 58.61	G
	ATOM	2521		2 GLC		7	37.316	0.281	14.299	1.00 73.45	G
	ATOM	2522		L GLC		7	37.655	-0.758	15.222	1.00 72.78	G
	ATOM	2523		GLC		7	36.592	-1.856	15.157	1.00 72.98	G
20	MOTA	2524	014	GLC	G	7	35.320	-1.299	15.498	1.00 73.88	G
	ATOM	2525	C15	GLC	G	7	36.924	-2.989	16.134	1.00 73.66	G [°]
	ATOM	2526	016	GLC	G	7	36.972	-2.493	17.478	1.00 75.38	G
	ATOM	2527	012	GLC	G	8	51.921	21.898	5.908	1.00 62.51	Ğ
	ATOM	2528	C11	GLC	G	8	52.447	20.871	5.063	1.00 63.42	Ğ
25	ATOM	2529	C13	GLC	: G	8	51.476	20.597	3.908	1.00 64.28	G
	ATOM	2530		GLC		8	51.297	21.794	3.150	1.00 66.28	G
	ATOM	2531		GLC		8	50.121	20.137	4.448	1.00 64.49	G
	ATOM	2532		GLC		8	49.233	19.886	3.357	1.00 64.49	G
	ATOM	2533		GLC		10	36.044	37.499			
30	ATOM	2534		. GLC		10			29.523	1.00 56.89	G
50	ATOM	2535					35.164	36.645	30.259	1.00 56.97	G
				GLC		10	33.849	36.489	29.494	1.00 56.11	.G
	ATOM	2536	014			10	33.248		29.308	1.00 56.44	G
	ATOM	2537		GLC		10	32.900	35.580	30.277	1.00 55.84	G
~=	ATOM	2538		GLC		10	31.674	35.442	29.557	1.00 55.39	G
35	ATOM	2539		ATP		1	46.280	25.658	5.170	1.00 51.49	N
	ATOM	2540	PG	ATP		1	46.464	25.053	3.691	1.00 52.22	N
	ATOM	2541	01G	ATP	N	1	47.406	23.911	3.763	1.00 51.41	N
	ATOM	2542	02G	ATP	N	1	46.794	26.182	2.784	1.00 52.07	N
	ATOM	2543	03B	ATP	N	1	44.976	24.513	3.344	1.00 51.01	N
40	MOTA	2544	PB	ATP	N	1	44.560	22.969	3.605	1.00 50.20	'N
	ATOM	2545	01B	ATP	N	1	43.083	22.898	3.669	1.00 49.41	N
	ATOM	2546	02B	ATP	N	1	45.345	22.474	4.766	1.00 50.34	N
	ATOM	2547	03A	ATP	N	1	45.070	22.231	2.255	1.00 47.77	N
	ATOM	2548	PA	ATP		1	45.075	20.613	2.121	1.00 42.84	N
45	MOTA	2549		ATP		1	45.547	20.291		1.00 43.81	N
	ATOM	2550		ATP		ī	45.807	20.035	3.270	1.00 45.03	
	ATOM	2551		ATP		ī	43.516	20.223		1.00 41.73	N
	ATOM	2552		ATP		1			2.245		N
	ATOM	2553		ATP			42.528	20.925	1.489	1.00 37.57	N
50						1	41.127	20.379	1.776	1.00 39.45	N
50	MOTA	2554		ATP		1	40.907	19.024	1.279	1.00 37.72	N
	ATOM	2555		ATP		1	40.777	20.321	3.251	1.00 38.48	N
	ATOM	2556		ATP		1	40.360	21.615	3.697	1.00 40.42	N
	ATOM	2557		ATP		1	39.608	19.374	3.270	1.00 37.58	N
	ATOM	2558		ATP		1	38.410	20.076	2.924	1.00 35.98	N
55	MOTA	2559		ATP		1	39.939	18.346	2.173	1.00 35.55	N
	MOTA	2560	N9	ATP		1	40.628	17.156	2.747	1.00 31.76	N
	ATOM	2561	C8	ATP	N	1	41.864	17.126	3.274	1.00 30.49	N
	MOTA	2562	N7	ATP		1	42.143	15.877	3.667	1.00 29.75	N
	ATOM	2563	C5	ATP	N	1	41.088	15.118	3.390	1.00 27.49	N

	ATOM	2564	C4	ATP N	1	40.125	15.925	2.810	1.00 30.02	N
	ATOM	2565	N3	ATP N	1	38.937	15.389	2.431	1.00 27.11	N
	MOTA	2566	C2	ATP N	1	38.679	14.085	2.615	1.00 25.62	N
	ATOM	2567	N1	ATP N	1	39.597	13.283	3.175	1.00 21.76	N
5	ATOM	2568	C6	ATP N	1	40.800	13.768	3.571	1.00 23.90	N
	ATOM	2569	N6	ATP N	1	41.698	12.964	4.127	1.00 21.94	N
	MOTA	2570	s	SO4 I	1	58.680	8.493	-0.639	1.00 56.05	I
	MOTA	2571	01	SO4 I	1	57.956	7.875	0.483	1.00 58.83	I
	ATOM .	2572	02	SO4 I	1	57.886	9.607	-1.188	1.00 57.04	1
10	MOTA	2573	03	SO4 I	1	58.906	7.478	-1.683	1.00 57.47	I
	ATOM	2574	04	SO4 I	1	59.976	9.008	-0.156	1.00 57.51	I
	MOTA	2575	S	SO4 I		39.339	4.855	7.057	1.00 84.24	I
	ATOM	2576	01	SO4 I	_	39.390	6.175	7.711	1.00 85.02	I
	MOTA	2577	02	SO4 I		40.101	4.897	5.797	1.00 84.75	Ī
15	MOTA	2578	03	SO4 I	2	37.936	4.506	6.766	1.00 84.94	I
	ATOM	2579	· 04	SO4 I		39.931	3.842	7.954	1.00 84.44	I
	MOTA	2580	S	SO4 I	3	38.987	-2.256	3.310	1.00 58.58	I
	MOTA	2581	01	SO4 I	_	37.734	-1.675	3.827	1.00 59.11	I
	ATOM	2582	02	SO4 I	-	39.460	-1.454	2.172	1.00 59.91	I
20	MOTA	2583	03	SO4 I	-	38.743	-3.640	2.866	1.00 60.97	I
	MOTA	2584	Ο4.	SO4 ·I	3	40.014	-2.260	4.369	1.00 59.58	I
	MOTA	2585	S	SO4 I	4	34.397	5.289	30.981	1.00 64.34	I
	ATOM	2586	01	SO4 I	4	33.627	6.528	30.742	1.00 60.43	I
	MOTA ·	2587	02	SO4 · I	4	34.337	4.427	29.782	1.00 60.11	I
25	ATOM	2588	03	SO4 I	4	33.816	4.572	32.133	1.00 64.39	I
	ATOM	2589	04	SO4 I	_	35.806	5.626	31.277	1.00 63.55	I
	MOTA	2590	S	SO4 I		55.074	-6.984	-3.711	1.00 75.40	I
	ATOM	2591	01	SO4 I	5	54.657	-7.518	-2.399	1.00 74.66	I '
	MOTA	2592	02	SO4 I	5	54.209	-5.845	-4.065	1.00 74.96	I
30	MOTA	2593	03	SO4 I	5	54.950	-8.034	-4.742	1.00 74.22	· I
	ATOM	2594	04	SO4 I	5	56.477	-6.532	-3.633	1.00 75.15	I
	MOTA	2595	02	PO4 P		57.362	24.998	13.149	1.00 66.76	P
	MOTA	2596	03	PO4 P		59.399	26.166	13.761	1.00 66.89	P
	ATOM	2597	04	PO4 P		57.761	25.606	15.462	1.00 67.43	· P
35	MOTA	2598	01	PO4 P		57.264	27.325	13.818	1.00 65.91	P
	MOTA	2599	P	PO4 P	100	57.947	26.025	14.048	1.00 66.69	P
	END									

## **Example 5: PDK1 fragments**

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We produced constructs for expression of different forms of PDK1 in bacteria. The constructs were either in TRC vectors, pET-15b vector and pGEX expression vector to enable the expression of GST fused N-terminally to PDK1. PDK1 expressed from pGEX 51-556 (ie residues 51 to 556 of PDK1) was found to be highly degraded.

PDK1 protein was also expressed with N-terminal His tags from vector TRC comprising PDK1 sequences 51-556, 51-404 and 1-360, or pET15b 51-404 and tested for expression levels and activity. The expression was generally low, around 0.2 mg/L culture. The specific activity was lower than the His-tagged 51-556 protein purified from baculovirus cells. In the case of PDK1 51-404 expressed from pET-15b construct the level of expression turned out to be very variable. This was probably due to instability of the plasmid since we produced evidence that after a growth of 0.2 units of absorbance, (as measured in a spectrophotometer at 600 nm wavelength) the cells growing faster in the culture were actually not harbouring the plasmid with ampiciline resistance. The instability of the plasmid can be due to toxicity produced by basal expression of PDK1. Although production in bacteria was the theoretical best expression system to avoid heterogeneity due to the different extent of phosphorylation of the different phosphorylation sites in hPDK1, it was found that the protein was either degraded, expressed to low levels, had 5 times less specific activity, or was possibly toxic.

The His-tagged purified PDK1 51-556 protein obtained from baculovirus expression system was homogeneous as depicted by the appearance of one band after by SDS-PAGE analysis of a sample.

Nevertheless, the analysis after isoelectric focussing revealed a large smear of protein covering several units of pH. This analysis suggested that the protein was not homogeneous in terms of its isoelectric point, possibly due to the number of phosphorylation sites which were not homogeneously phosphorylated. This protein did not crystallise.

We purified to homogeneity a truncated His-Myc tagged PDK1 (51-404) which lacks the N-terminal 50 residues and the C-terminal 152 residues which include the PH domain. This protein, produced by a baculovirus expression system, had similar characteristics to the full length wild type PDK1 in terms of its activity towards the peptide substrate T308tide, its activation by the peptide PIFtide, and the binding to PIFtide (as analysed by BiaCore). The purified protein was screened for crystallisation conditions using Hampton Research kits (144 different conditions). Crystallisation conditions were screened with two concentrations of PDK1, in the presence or absence of PIFtide, Staurosporine, at 20°C and in the presence of PIFtide at 4°C. No protein crystals were observed after 6 months, suggesting that this construct was not suitable for forming crystals although all other characteristics were similar to wild type protein.

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The His-Myc PDK1 51-404 purified protein was also subjected to protease treatments in order to obtain a protease-insensitive molecule for increasing the chances of obtaining a shorter, stable variant of PDK1. Different protease treatments were tested. Treatment with Glu-C produced a polypeptide of approximately 38 KDa which was stable. This PDK1 protein was active and lacked the His-tag and part of the Myc-tag, and possibly part of the C-terminal residues. This protein was also set up for crystallography screenings. Some crystals were obtained using this preparation after 4 months, but they were not followed up.

A protein kinase corresponding to residues PDk1 51-387 was also produced, in an identical vector to that used to produce the protein PDK1 51-359. Interestingly, this protein was similar to wild type and PDK1 51-404, but had extreme problems for concentration using conventional methods. The protein could not be concentrated further than 2.5 mg/ml, and no crystals were obtained using this construct.

The PDK1 protein that finally crystallised is lacking the first 50 aminoacids and was constructed to end at position 359. This protein was stable in the absence of the PH domain and aminoacids that in hPDK1 link the catalytic domain with the PH domain. The construct PDK1 51-359 was also short enough that no other described phosphorylation sites besides activation loop phosphorylation site 241 were present.

## CLAIMS .

1. A method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

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2. The method of claim 1 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues 51 to 359 of full length human PDK1 or a fusion thereof.

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3. The method of claim 2 wherein the three-dimensional structure (or part thereof) is determined for a polypeptide consisting of residues 51 to 359 of full length human PDK1 and the amino acid sequence Gly-Pro preceding the methionine corresponding to Met51 of human PDK1.

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4. The method of claim 1 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is a three-dimensional structure (or part thereof) determined for a polypeptide

consisting of residues 71 to 359 of full length human PDK1 or a fusion thereof.

- 5. The method of any one of the preceding claims wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is obtainable by X-ray analysis of a crystal obtainable using a mother liquor solution comprising ammonium sulphate.
- 6. The method of claim 5 wherein the mother liquor solution is of pH 7 to 9.
  - 7. The method of claim 6 wherein the mother liquor solution is of pH 8.5.
- 8. The method of any one of claims 5 to 7 wherein the mother liquor solution comprises ATP.
  - 9. The method of any one of claims 1 to 3, 5 to 8 wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 structure is that represented by the structure co-ordinates shown in Examples 2, 3 or 4, or a structure modelled on such structure co-ordinates.

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10. The method of any one of the preceding claims wherein the molecule is predicted to bind to a region of the structure termed the "PIF binding pocket" (formed by residues including residues Lys115, Ile118, Ile119 on the  $\alpha B$  helix, Val124, Val127 on the  $\alpha C$  helix and Leu 155 on  $\beta$ -sheet 5 of full length human PDK1, or equivalent residues), the "phosphate binding pocket" (formed by residues including residues Lys76, Arg 131, Thr 148 and Gln150 of full length human PDK1, or equivalent residues) and/or the

α C helix (residues equivalent to 123-136 of full length human PDK1), or interacting regions.

11. The method of any of the preceding claims wherein the compound is for modulating the protein kinase activity of PDK1 towards PKB or other PH-domain-comprising/phosphoinositide-binding substrate of PDK1.

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- 12. The method of any one of claims 1 to 10 wherein the compound is for modulating the protein kinase activity of PDK1 towards SGK, S6K or other substrate of PDK1 whose phosphorylation by PDK1 is promoted by phosphorylation of the substrate on the Ser/Thr of the "hydrophobic motif" FXXFS/TY.
- 13. A method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally

also the hydrophobic pocket and/or  $\alpha C$  helix or region interacting therewith, is selected.

- 14. The method of claim 13 wherein the protein kinase is an isoform of Serum and Glucocorticoid stimulated protein kinase (SGK), Protein Kinase B (PKB), p70 S6 kinase, p90 RSK, PKC isoforms (for example PKCα, PKCδ, PKCζ), PRK1, PRK2, MSK1 or MSK2.
- 15. The method of claim 13 or 14 wherein the three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith is a structure modelled on the basis of a three-dimensional structure as defined in any one of claims 1 to 9.
- 16. The method of any one of the preceding claims further comprising the step of synthesising, purifying and/or formulating the compound.
  - 17. A method for assessing the activation state of a structure for a protein kinase, wherein the structure is analysed using principle component analysis of the structure co-ordinates.

- 18. The method of claim 17 wherein the activation state of the structure is classified as "open", "closed" or "intermediate".
- 19. A mutated protein kinase, wherein the protein kinase before mutation has a hydrophobic pocket in the position equivalent to the hydrophobic pocket (PIF-binding pocket) of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further has a phosphate binding pocket in the

position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, and wherein one or more residues equivalent to Ile118, Val124, Val127, Lys76 or Thr148 forming part of the hydrophobic pocket or phosphate binding pocket of the protein kinase is mutated.

- 20. The mutated protein kinase of claim 19 wherein the protein kinase is PDK1.
- 10 21. The mutated protein kinase of claim 19 wherein the protein kinase is SGK, PKB or p70 S6 kinase.
  - 22. The mutated protein kinase of any one of claims 19 to 21 wherein the residue at the position equivalent to residue Lys76 of PDK1 is mutated to an Ala.

- 23. A polynucleotide encoding a mutated protein kinase according to any one of claims 19 to 22.
- 24. A polynucleotide according to claim 23 suitable for expressing a mutated protein kinase according to any one of claims 19 to 22.
  - 25. A host cell comprising a polynucleotide according to claim 23 or 24.
- 26. A method of making a mutated protein kinase according to any one of claims 19 to 22, the method comprising culturing a host cell according to claim 25 which expresses said mutated protein kinase and isolating said mutated protein kinase.
- 30 27. A mutated protein kinase obtainable by the method of claim 26.

- 28. A method of identifying a compound that modulates the protein kinase activity of a protein kinase as defined in claim 19 (for example PDK1), comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to a mutated protein kinase according to any one of claims 19 to 22, 27.
- 29. The method of claim 28 further comprising the step of determining the effect of the compound on the protein kinase activity of, or ability of the compound to bind to, the protein kinase (for example PDK1) which is not mutated as defined in any one of claims 19 to 22.
- 30. An antibody reactive with the phosphate binding pocket of PDK1 or other protein kinase as defined in claim 19; or an antibody reactive with PDK1 or other protein kinase as defined in claim 19 but not with the said protein kinase mutated at the phosphate binding site, or *vice versa*..
  - 31. A method for preparing or selecting an antibody according to claim 30 wherein the antibody is prepared or selected against a said protein kinase (for example PDK1) unmutated at the phosphate binding site and a said protein kinase mutated at the phosphate binding site.
- 32. A kit of parts comprising (1) a mutated protein kinase (for example mutated PDK1) according to any one of claims 19 to 22, 27 (2) the corresponding protein kinase (for example PDK1) which is not mutated as defined in any one of claims 19 to 22.
  - 33. A compound identified or identifiable by any one of claims 1 to 16, 28 or 29.

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- 34. The compound of claim 33 wherein the compound comprises an antibody or RNA molecule.
- 35. A compound according to claim 33 or 34, mutated protein kinase according to any one of claims 19 to 22, 27 or polynucleotide according to claim 23 or 24, for use in medicine.
- 36. Use of a compound, mutated protein kinase or polynucleotide as defined in claim 35 in the manufacture of a medicament for the treatment of
   a patient in need of modulation of signalling by a protein kinase as defined in claim 19, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling.
- 15 37. A method of treating a patient in need of modulation of signalling by a protein kinase as defined in claim 19, for example PDK1, SGK, PKB or p70 S6 kinase, for example insulin signalling pathway and/or PDK1/PDK2/SGK/PKB/p70 S6 kinase/PRK2/PKC signalling, wherein the patient is administered an effective amount of a compound, mutated protein kinase or polynucleotide as defined in claim 35.

## ABSTRACT

A method for selecting or designing a compound for modulating the activity of phosphoinositide dependent protein kinase 1 (PDK1), the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the protein kinase catalytic domain of PDK1, wherein a three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is compared with a three-dimensional structure of a compound, and a compound that is predicted to interact with the said protein kinase catalytic domain is selected, wherein the three-dimensional structure of at least a part of the protein kinase catalytic domain of PDK1 is a three-dimensional structure (or part thereof) determined for a polypeptide consisting of residues equivalent to residues 51 to 359 of full length human PDK1, or a fragment or fusion thereof.

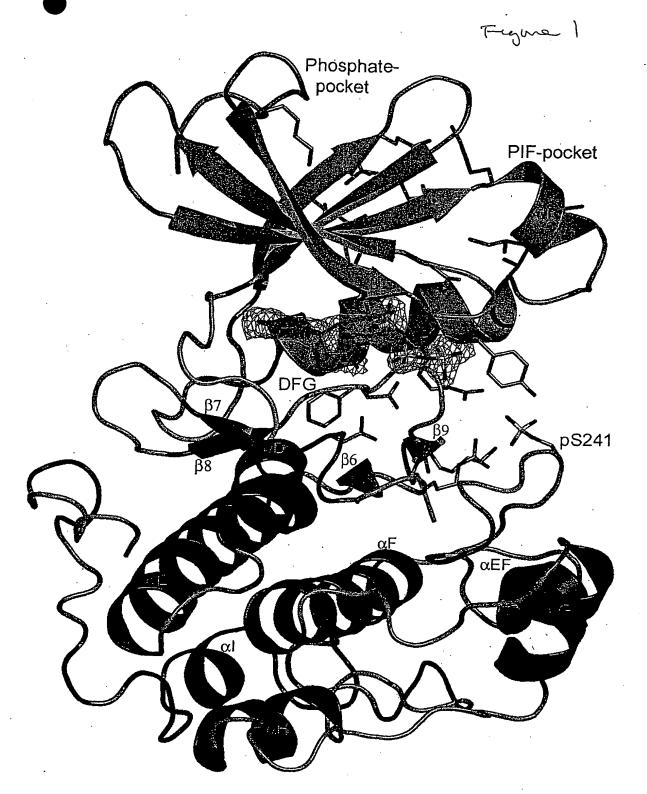
A method for selecting or designing a compound for modulating the activity of a hydrophobic pocket (PIF binding pocket)-containing protein kinase having a hydrophobic pocket in the position equivalent to the hydrophobic pocket of human PDK1 that is defined by residues including Lys115, Ile118, Ile119, Val124, Val127 and/or Leu155 of full-length human PDK1 and further having a phosphate binding pocket in the position equivalent to the phosphate binding pocket of human PDK1 that is defined by residues including Lys76, Arg131, Thr148 and/or Gln150, the method comprising the step of using molecular modelling means to select or design a compound that is predicted to interact with the said hydrophobic pocket-containing protein kinase, wherein a three-dimensional structure of a compound is compared with a three-dimensional structure of the said phosphate binding pocket and optionally also the hydrophobic pocket and/or αC helix or region interacting therewith, and a compound that is predicted to interact with the said phosphate binding pocket and optionally

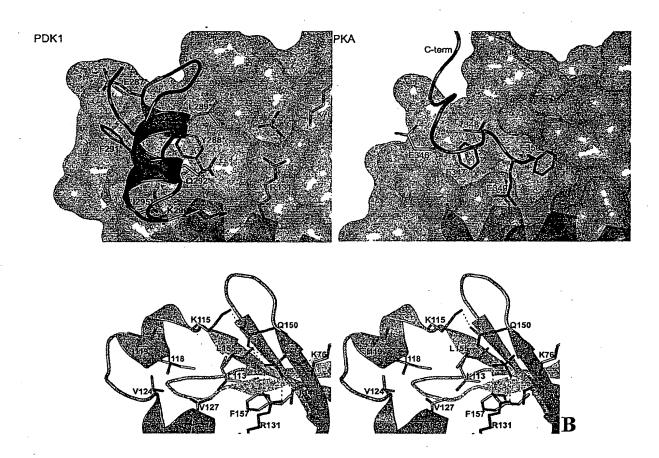
also the hydrophobic pocket and/or  $\alpha C$  helix or region interacting therewith, is selected.

FIGURE 1.

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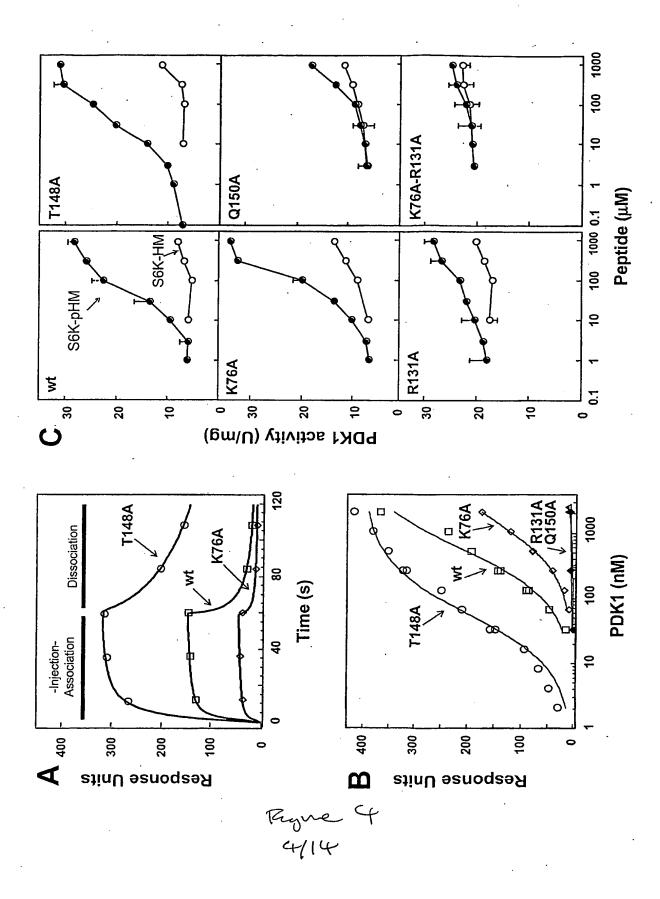


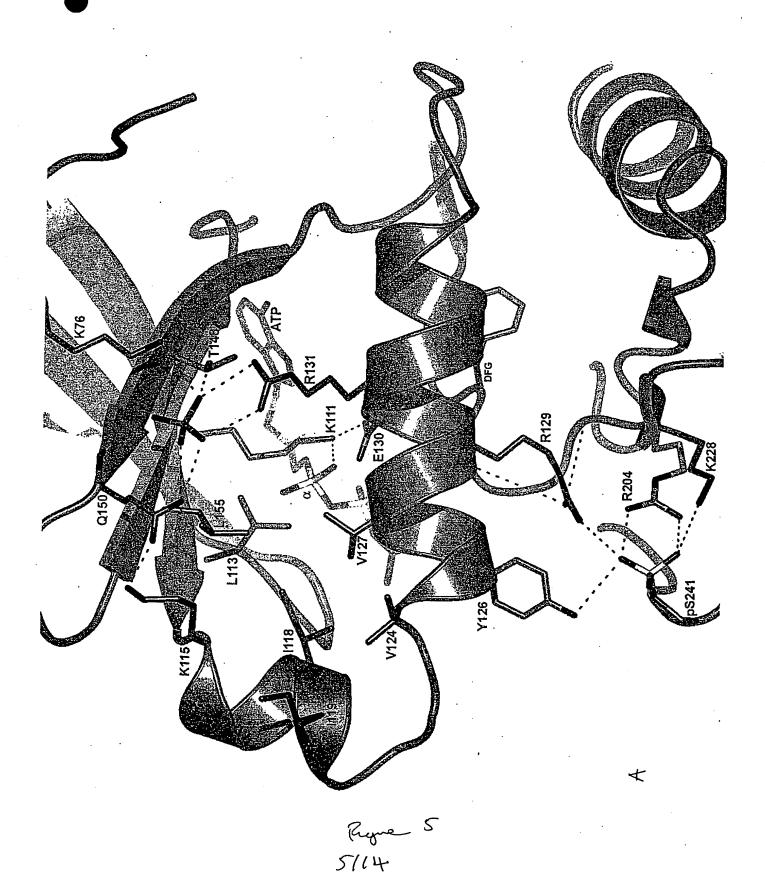


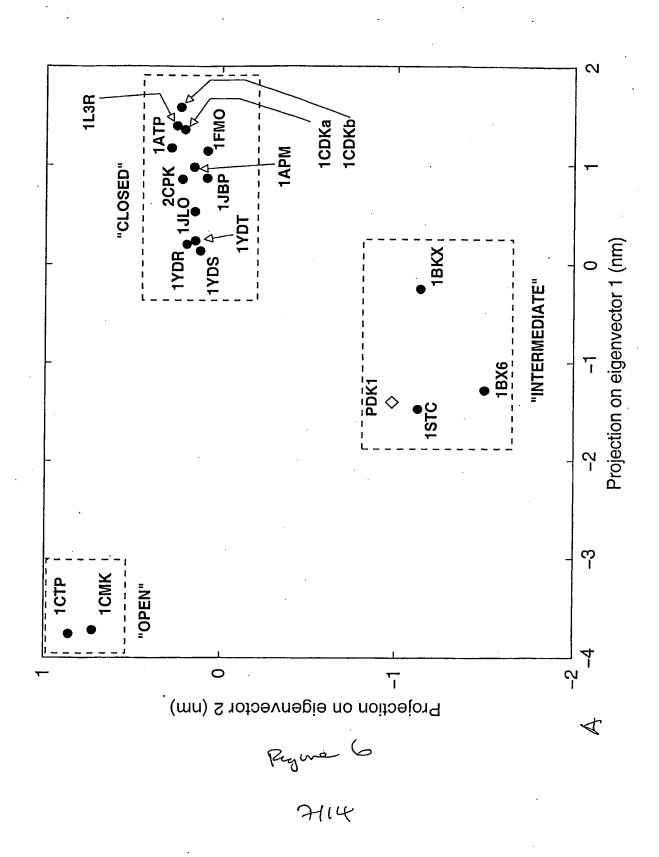
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08 05	KREWENKLENKYPYVTREWDYNNSKENDHD KOWENNIKLKOMEHTLNEMRREMDAMNPP OCE	Y TAELVSALEYLHS KOMIRD LKPEN YAAQIVL TFEYLHS L DMIYRD LKPEN	のF 200 TEKSACKSSDLWALGC網IYOMVAGLD LSKGYNKAVDWALGV網IYEMAAGYP	d sw LGCEEMEGYGP版KAHP院EEGVTWENE PGN-LKNGVND流KNHKWEAUTDWIA	
β2 β3 β3 100 110 110 110 110 110 110 110 110 11	MULAKE LANSKEYAMKILIM MULVKHKE SGNHYAMKILIM CD	YAKNGE BLKY AR MIGSPOET CTRF YVAGGE BFSHTRATGRESBPHARP	SPESKOARANÝFVGTAOVÝSPEŇÍ	OH 300 P E WE P P K A KO LIVE K L L V WO A T K R I E DS HIGS S D L KO L SR N L D Q WO L T K R I	
18 00 00 00 00 00 00 00 00 00 00 00 00 00	1 P S G N T N C L	180 FLVKLYEEES PKDNSNLYEG 以S FLVKEEE PS PKDNSNLYNVEE	は	PERAC SEYLING KLEYD PERAD OP 101 SEKT SGKVR	TEN O O H -
7.1	32	141	211 172	281	351
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## Lysits

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		₩ Heng Figure 7-(page 1 of 6)
p70S6Kalpha	104	KVFQVRKVTGANTGKIFAMKVLKKAMIVRNAKDTAHTKAERNILEEVKH-PFI
p70S6Kbeta	93	KVFQVRKVQGTNLGKIYAMKVLRKAKIVRNAKDTAHTRAERNILESVKH-PFI
p90RSK1	81	KVFLVKKISGSDARQLYAMKVLKKATLKVRDRVRTKMERDILVEVNH-PFI
p90RSK2	81	KVFLVKKISGSDARQLYAMKVLKKATLKVRDRVRTKMERDILVEVNH-PFI
p90RSK3	72	KVFLVRKVKGSDAGQLYAMKVLKKATLKVRDRVRSKMERDILAEVNH-PFI
MSK1	62	KVFLVRKISGHDTGKLYAMKVLKKATIVQKAKTTEHTRTERQVLEHIRQSPFL
MSK2	30	KVFLVRKAGGHDAGKLYAMKVLRKAALVQRAKTQEHTRTERSVLELVRQAPFL
PKBalpha		KVILVKEKATGRYYAMKILKKEVIVAKDEVA-HTLTENRVLQNSRHPFL
PKBbeta		KVILVREKATGRYYAMKILRKEVIIAKDEVA-HTVTESRVLQNTRHPFL
PKBgamma	161	KVILVREKASGKYYAMKILKKEVIIAKDEVA-HTLTESRVLKNTRHPFL
PRK1		KVLLSEFRPSGELFAIKALKKGDIVARDEVE-SLMCEKRILAAVTSAGHPFL
PRK2	670	KVLLAEYKNTNEMFAIKALKKGDIVARDEVD-SLMCEKRIFETVNSVRHPFL
SGK1		KVLLARHKAEEVFYAVKVLQKKAILKKKEEK-HIMSERNVLLKNVKHPFL
· SGK3	108	KVLLAKRKLDGKFYAVKVLQKKIVLNRKEQK-HIMAERNVLLKNVKHPFL
SGK2		KVLLAKRKSDGAFYAVKVLQKKSILKKKEQS-HIMAERSVLLKNVRHPFL
PKCbeta	355	KVMLSERKGTDELYAVKILKKDVVIQDDDVE-CTMVEKRVLALPGKPPFL
PKCbetall	355	KVMLSERKGTDELYAVKILKKDVVIQDDDVE-CTMVEKRVLALPGKPPFL
PKCalpha.	352	KVMLADRKGTEELYAIKILKKDVVIQDDDVE-CTMVEKRVLALLDKPPFL
PKCgamma	364	KVMLAERRGSDELYAIKILKKDVIVQDDDVD-CTLVEKRVLALGGRGPGGRPHFL
PKCzeta	257	KVLLVRLKKNDQIYAMKVVKKELVHDDEDID-WVQTEKHVFEQASSNPFL
PKCiota	258	KVLLVRLKKTDRIYAMKVVKKELVNDDEDID-WVQTEKHVFEQASNHPFL
<b>PKCdelta</b>	362	KVLLGELKGRGEYSAIKALKKDVVLIDDDVE-CTMVEKRVLTLAAENPFL
PKAgamma	57	RVMLVRHQETGGHYAMKILNKQKVVKMKQVE-HILNEKRILQAIDFPFL
PDK1	95	TVVLARELATSREYAIKILEKRHIIKENKVP-YVTRERDVMSRLDHPFF

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		Giniso +	V Leulss	Figure 7 (page 2 of 6)
p70S6Kalpha	156	VDLIYAFQTGGK	LYLILEYLSGGELFMQLEREGI	VDLIYAFQTGGKLYLILEYLSGGELFMQLEREGIFMEDTACFYLAEISMALGHLHQ-KGI
p70S6Kbeta	145	VELAYAFQTGGK	LYLILECLSGGELFTHLEREGI	VELAYAFQTGGKLYLILECLSGGELFTHLEREGIFLEDTACFYLAEITLALGHLHS-QGI
p90RSK1	131	VKLHYAFQTEGK	LYLILDFLRGGDLFTRLSKEVM	VKLHYAFQTEGKLYLILDFLRGGDLFTRLSKEVMFTEEDVKFYLAELALALDHLHS-LGI
p90RSK2	131	VKLHYAFQTEGK	LYLILDFLRGGDLFTRLSKEVM	VKLHYAFQTEGKLYLILDFLRGGDLFTRLSKEVMFTEEDVKFYLAELALAHHS-LGI
p90RSK3	122	VKLHYAFQTEGK	LYLILDFLRGGDLFTRLSKEVM	VKLHYAFQTEGKLYLILDFLRGGDLFTRLSKEVMFTEEDVKFYLAELALALDHLHS-LGI
MSK1	115	VTLHYAFQTETK	LHLILDYINGGELFTHLSQRER	VTLHYAPQTETKLHLILDYINGGELFTHLSQRERFTEHEVQIYVGEIVLALEHLHK-LGI
MSK2	83	VTLHYAFQTDAK	LHLILDYVSGGEMFTHLYQRQY:	VTLHYAFQTDAKLHLILDYVSGGEMFTHLYQRQYFKEAEVRVYGGEIVLALEHLHK-LGI
<b>PKBalpha</b>	211	TALKYSFQTHDR	LCFVMEYANGGELFFHLSRERV	TALKYSPQTHDRLCFVMEYANGGELFFHLSRERVFSEDRARFYGAEIVSALDYLHSEKNV
PKBbeta	213	TALKYAFQTHDR	LCFVMEYANGGELFFHLSRERV	TALKYAFQTHDRLCFVMEYANGGELFFHLSRERVFTEERARFYGAEIVSALEYLHS-RDV
PKBgamma	209	TSLKYSFQTKDR	LCFVMEYVNGGELFFHLSRERV.	TSLKYSFQTKDRLCFVMEYVNGGELFFHLSRERVFSEDRTRFYGAEIVSALDYLHS-GKI
PRK1	619	VNLFGCFQTPEH	VCFVMEYSAGGDLMLHIHSD-V	VNLFGCFQTPEHVCFVMEYSAGGDLMLHIHSD-VFSEPRAIFYSACVVLGLQFLHE-HKI
PRK2	721	VNLFACFQTKER	VCFVMEYAAGGDLMMHIHTD-V.	VNLFACFQTKEHVCFVMEYAAGGDLMMHIHTD-VFSEPRAVFYAACVVLGLQYLHE-HKI
SGK1	160	VGLHFSFQTADK	LYFVLDYINGGELFYHLQRERC	VGLHFSFQTADKLYFVLDYINGGELFYHLQRERCFLEPRARFYAAEIASALGYLHS-LNI
SGK3	157	VGLHYSFQTTEK	LYFVLDFVNGGELFFHLQRERS	VGLHYSFQTTEKLYFVLDFVNGGELFFHLQRERSFPEHRARFYAAEIASALGYLHS-IKI
SGK2	157	VGLRYSFQTPER	LYFVLDYVNGGELFFHLORERR	VGLRYSFQTPEKLYFVLDYVNGGELFFHLQRERRFLEPRARFYAAEVASAIGYLHS-LNI
PKCbeta	404	TQLHSCFQTMDR	LYFVMEYVNGGDLMYHIQQVGR	TQLHSCFQTMDRLYFVMEYVNGGDLMYHIQQVGRFKEPHAVFYAAEIAIGLFFLQS-KGI
PKCbetall	404	TQLHSCFQTMDR	LYFVMEYVNGGDLMYHIQQVGR	TQLHSCFQTMDRLYFVMEYVNGGDLMYHIQQVGRFKEPHAVFYAAEIAIGLFFLQS-KGI
PKCalpha	401	TQLHSCFQTVDR	LYFVMEYVNGGDLMYHIQQVGK	TQLHSCFQTVDRLYFVMEYVNGGDLMYHIQQVGKFKEPQAVFYAAEISIGLFFLHK-RGI
PKCgamma	418	TQLHSTFQTPDR	LYFVMEYVTGGDLMYHIQQLGK	TQLHSTFQTPDRLYFVMEYVTGGDLMYHIQQLGKFKEPHAAFYAAEIAIGLFFLHN-QGI
PKCzeta	306	VGLHSCFQTTSR	LFLVIEYVNGGDLMFHMQRQRK	VGLHSCFQTTSRLFLVIEYVNGGDLMFHMQRQRKLPEEHARFYAAEICIALNFLHE-RGI
PKCiota	307	VGLHSCFQTESF	LFFVIEYVNGGDLMFHMQRQRK	VGLHSCFQTESRLFFVIEYVNGGDLMFHMQRQRKLPEEHARFYSAEISLALNYLHE-RGI
PKCdelta	411	THLICTFOTKDE	LFFVMEFLNGGDLMYHIQDKGR	THLICTFQTKDHLFFVMEFLNGGDLMYHİQDKGRFELYRATFYAAEIMCGLQFLHS-KGI

VKLQFSFKDNSYLYLVMEYVPGGEMFSRLQRVGRFSEPHACFYAAQVVLAVQYLHS-LDL

105

**PKAgamma** 

PDK1

143

VKLYFTFQDDEKLYFGLSYAKNGELLKYIRKIGSFDETCTRFYTAEIVSALEYLHG-KGI

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## Figure 7 (page 3 of 6)

			)
p70S6Kalpha	215 IN	IYRDLKPENIMLNHQGHVKLTDFGLCKESIHDGT	-VTHTFCGTIEYMAPEILMRSG
p70S6Kbeta	204 IN	IYRDLKPENIMLSSQGHIKLTDFGLCKESIHEGA	-VTHTFCGTIEYMAPEILVRSG
p90RSK1	190 IN	IYRDLKPENILLDEEGHIKLTDFGLSKESIDHEK	KAYSFCGTVEYMAPEVVNRRG
p90RSK2	190 IN	IYRDLKPENILLDEEGHIKLTDFGLSKESIDHEK	KAYSFCGTVEYMAPEVVNRRG
p90RSK3	181 IX	IYRDLKPENILLDEEGHIKITDFGLSKEAIDHDK	RAYSFCGTIEYMAPEVVNRRG
MSK1	174 IY	IYRDIKLENILLDSNGHVVLTDFGLSKEFVADET	ERAYSFCGTIEYMAPDIVRGGDSG
MSK2	142 IY	IYRDLKLENVLLDSEGHIVLTDFGLSKEFLTEEK	ERTFSFCGTIEYMAPELIR-SKTG
PKBalpha	271 VY	VYRDLKLENLMLDKDGHIKITDFGLCKEGIKDGA	-TMKTFCGTPEYLAPEVLEDND
. PKBbeta	272 VY	VYRDIKLENLMLDKDGHIKITDFGLCKEGISDGA	-TMKTFCGTPEYLAPEVLEDND
PKBgamma	268 VY	VYRDLKLENLMLDKDGHIKITDFGLCKEGITDAA	-TMKTFCGTPEYLAPEVLEDND
PRK1	737 W	VYRDLKLDNLLLDTEGYVKIADFGLCKEGMGYGD	RTSTFCGTPEFLAPEVLTDTS
PRK2	779 W	VYRDLKLDNLLLDTEGFVKIADFGLCKEGMGYGD	RTSTFCGTPEFLAPEVLTETS
SGK1	219 VY	VYRDLKPENILLDSQGHIVLTDFGLCKENIEHNS	-TTSTFCGTPEYLAPEVLHKQP
SGK3	216 VA	VYRDLKPENILLDSVGHVVLTDFGLCKEGIAISD	-TTTTFCGTPEYLAPEVIRKQP
SGK2	216 IY	IYRDLKPENILLDCQGHVVLTDFGLCKEGVEPED	-TTSTFCGTPEYLAPEVLRKEP
PKCbeta	463 IY	IYRDLKLDNVMLDSEGHIKIADFGMCKENIWDGV	-TTKTFCGTPDYIAPEIIAYQP
PKCbetaII	463 IY	IYRDLKLDNVMLDSEGHIKIADFGMCKENIWDGV	-TTKTFCGTPDYIAPEIIAYQP
PKCalpha	460 IY	IYRDLKLDNVMLDSEGHIKIADFGMCKEHMMDGV	-TTRTFCGTPDYIAPELIAYQP
PKCgamma	477 IY	IYRDLKLDNVMLDAEGHIKITDFGMCKENVFPGT	-TTRTFCGTPDYIAPEIIAYQP
PKCzeta	365 IY	IYRDLKLDNVLLDADGHIKLTDYGMCKEGLGPGD	-TTSTFCGTPNYIAPEILRGEE
PKCiota	366 IY	IYRDLKLDNVLLDSEGHIKLTDYGMCKEGLRPGD	-TTSTFCGTPNYIAPEILRGED
PKCdelta	470 IY	IYRDLKLDNVLLDRDGHIKIADFGMCKENIFGES	-RASTFCGTPDYIAPEILQGLK
PKAgamma	164 IE	IHRDLKPENLLIDQQGYLQVTDFGFAKRVKG	-RTWTLCGTPEYLAPEIILSKG
PDK1	202 IF	IHRDLKPENILLNEDMHIQITDFGTAKVLSPESKQA-RANSFVGTAQYVSPELLT-	-RANSFVGTAQYVSPELLTEKS

## Figure 7 (page 4 of 6)

•			(0 to 1 29nd) 2 mg
p70S6Kalpha	270	HNRAVDWWSLGALMYDMLTGAPPFTGE	NRKKTIDKILKCKLNLPPYLTQEA
p70S6Kbeta	259	HNRAVDWWSLGALMYDMLTGSPPFTAE	NRKKTMDKIIRGKLALPPYLTPDA
p90rsk1	245	HTQSADWWSFGVLMFEMLTGTLPFQGK	DRKETMTMILKAKLGMPQFLSPEA
p90RSK2	4	HTQSADWWSFGVLMFEMLTGTLPFQGK	DRKETMTMILKAKLGMPQFLSPEA
p90rsk3	S	HTQSADWWSFGVLMFEMLTGSLPFQGK	DRKETMALILKAKLGMPQFLSGEA
MSK1	232	HDKAVDWWSLGVLMYELLTGASPFTVDG	EKNSQAEISRRILKSEPPYPQEMSALA
MSK2	199	HGKAVDWWSLGILLFELLTGASPFTLEG	ERNTQAEVSRRILKCSPPFPPRIGPVA
PKBalpha	326	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HEKLFELILMEEIRFPRTLGPEA
PKBbeta	327	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HERLFELILMEEIRFPRTLSPEA
PKBgamma	323	YGRAVDWWGLGVVMYEMMCGRLPFYNQD	HEKLFELILMEDIKFPRTLSSDA
PRK1		YTRAVDWWGLGVLLYEMLVGESPFPGDD	EEEVFDSIVNDEVRYPRFLSAEA
PRK2	834	YTRAVDWWGLGVLIYEMLVGESPFPGDD	EEEVFDSIVNDEVRYPRFLSTEA
SGK1	274	YDRTVDWWCLGAVLYEMLYGLPPFYSRN	TAEMYDNILNKPLQLKPNITNSA
SGK3	271	YDNTVDWWCLGAVLYEMLYGLPPFYCRD	VAEMYDNILHKPLSLRPGVSLTA
SGK2	271	YDRAVDWWCLGAVLYEMLHGLPPFYSQD	VSQMYENILHQPLQIPGGRTVAA
PKCbeta	518	YGKSVDWWAFGVLLYEMLAGQAPFEGED	EDELFQSIMEHNVAYPKSMSKEA
PKCbetaII	518	YGKSVDWWAFGVLLYEMLAGQAPFEGED	EDELFQSIMEHNVAYPKSMSKEA
PKCalpha	515	YGKSVDWWAYGVLLYEMLAGQPPFDGED	EDELFQSIMEHNVSYPKSLSKEA
PKCgamma	532	YGKSVDWWSFGVLLYEMLAGQPPFDGED	EEELFQAIMEQTVTYPKSLSREA
PKCzeta	420	YGFSVDWWALGVLMFEMMAGRSPFDIITD	-DNPDMNTEDYLFQVILEKPIRIPRFLSVKA
PKCiota	421	YGFSVDWWALGVLMFEMMAGRSPFDIVGSSDNPDQNTEDYLFQVILEKQIRIPRSLSVKA	NPDQNTEDYLFQVILEKQIRIPRSLSVKA
PKCdelta	525	YTFSVDWWSFGVLLYEMLIGQSPFHGDD	EDELFESIRVDTPHYPRWITKES
PKAgamma	216	YNKAVDWWALGVLIYEMAVGFPPFYADQ	PIQIYEKIVSGRVRFPSKLSSDL
PDK1	259	ACKSSDLWALGCIIYQLVAGLPPFRAGN	EYLIFQKIIKLEYDFPEKFFPKA

1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	1	
p/0S6Kalpha	321	RDLLKKLLKRNAASRLGAGPG-DAGEVQAHPFFRHINWEELLARKVEPPFKPLLQSE-
p70S6Kbeta	310	RDLVKKFLKRNPSQRIGGGPG-DAADVQRHPFFRHMNWDDLLAWRVDPPFRPCLQSE-
p90RSK1	296	QSLLRMLFKRNPANRLGAGPD-GVEEIKRHSFFSTIDWNKLYRREIHPPFKPATGRP-
p90RSK2	296	QSLLRMLFKRNPANRLGAGPD-GVEEIKRHSFFSTIDWNKLYRREIHPPFKPATGRP-
p90RSK3	287	QSLLRALFKRNPCNRLGAGID-GVEEIKRHPFFVTIDWNTLYRKEIKPPFKPALGRP-
MSK1		KDLIQRLLMKDPKKRLGCGPR-DADEIKEHLFFQKINWDDLAAKKVPAPFKPVIRDE-
MSK2	254	QDLLQRLLCKDPKKRLGAGPQ-GAQEVRNHPFFQGLDWVALAARKIPAPFRPQIRSE-
PKBalpha	377	KSLLSGLLKKDPKQRLGGGSE-DAKEIMQHRFFAGIVWQHVYEKKLSPPFKPQVTSE-
PKBbeta	378	KSLLAGLLKKDPKQRLGGGPS-DAKEVMEHRFFLSINWQDVVQKKLLPPFKPQVTSE-
PKBgamma	374	KSLLSGLLIKDPNKRLGGGPD-DAKEIMRHSFFSGVNWQDVYDKKLVPPFKPQVTSE-
PRK1	843	IGIMRRLLRRNPERRLGSSER-DAEDVKKQPFFRTLGWEALLARRLPPPFVPTLSGR-
PRK2	882	ISIMRRLLRRNPERRLGASEK-DAEDVKKHPFFRLIDWSALMDKKVKPPFIPTIRGR-
SGK1	325	RHLLEGLLQKDRTKRLGAKDDFMEIKSHVFFSLINWDDLINKKITPPFNPNVSGP-
SGK3	322	WSILEELLEKDRONRLGAKEDFLEIQNHPFFESLSWADLVQKKIPPPFNPNVAGP-
SGK2	322	CDLLQSLLHKDQRQRLGSKADFLEIKNHVFFSPINWDDLYHKRLTPPFNPNVTGP-
PKCbeta	569	VAICKGLMTKHPGKRLGCGPE-GERDIKEHAFFRYIDWEKLERKEIQPPYKPKARDK-
PKCbetall	569	VAICKGLMTKHPGKRLGCGPE-GERDIKEHAFFRYIDWEKLERKEIQPPYKPKACG
<b>PKCalpha</b>	266	VSICKGLMTKHPAKRLGCGPE-GERDVREHAFFRRIDWEKLENREIQPPFKPKVCG
PKCgamma	583	VAICKGFLTKHPGKRLGSGPD-GEPTIRAHGFFRWIDWERLERLEIPPFRPRPCG
PKCzeta	478	SHVLKGFLNKDPKERLGCRPQTGFSDIKSHAFFRSIDWDLLEKKQALPPFQPQITDD-
PKCiota	481	ASVLKSFLNKDPKERLGCHPQTGFADIQGHPFFRNVDWDMMEQKQVVPPFKPNISGE-
PKCdelta	576	KDILEKLFEREPTKRLGMTGNIKIHPFFKTINWTLLEKRRLEPPFRPKVKSP-
PKAgamma	267	KDLLRSLLQVDLTKRFGNLRN-GVGDIKNHKWFATTSWIAJYEKKVEAPFIPKYTGP-
PDK1	310	RDLVEKLLVLDATKRLGCEEMEGYGPLKAHPFFESVTWENLHQQTPPKLTAYLPAMSEDD

Figure 7 (p

,		de distribution de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la constant de la
p70S6Kalpha	377	EDVSQFDSKFTRQTPVDSPDDSTLSESANQVFLGFTYVAPSVLES-
p70S6Kbeta	366	EDVSQFDTRFTRQTPVDSPDDTALSESANQAFLGFTYVAPSVLDS-
p90RSK1	352	EDTFYFDPEFTAKTPKDSP-GIPPSANAHQLFRGFSFVAITSDDE-
p90RSK2	352	EDTFYFDPEFTAKTPKDSP-GIPPSANAHQLFRGFSFVAITSDDE-
p90RSK3	343	EDTFHFDPEFTARTPTDSP-GVPPSANAHHLFRGFSFVASSLIOEP
MSK1	343	LDVSNFAEEFTEMDPTYSPAALPQSSEKLFOGYSFVAPSILFKR
MSK2	310	LDVGNFAEEFTRLEPVYSPPGSPPPGDPRIFOGYSFVAPSILFDH
PKBalpha	433	TDTRYFDEEFTAQMITITPPDQDDSMECVDSERRPHFPQFSYSASSTA
PKBbeta	434	VDTRYFDDEFTAQSITITPPDRYDSLGLLELDQRTHFPOFSYSASIRE
PKBgamma	430	TDTRYFDEEFTAQTITITPPEKYDEDGMDCMDNERRPHFPOFSYSASGRF
PRK1	899	TDVSNFDEEFTGEAPTLSPPRDAR-PLTAAEOAAFLDFDFVAGGC
PRK2	941	EDVSNFDDEFTSEAPILTPPREPR-ILSEEEOEMFRDFDYTADWC
SGK1	380	NDLRHFDPEFTEEPVPNSIGKSPDSVLVTASVKEAAEAFLGFSYAPPT-DSFT
SGK3	377	1
SGK2	377	1
PKCbeta	625	- 1 - 1 - 1
PKCbetall	624	PDOEVIRNID
PKCalpha	621	QIN
PKCgamma	638	SID
PKCzeta	535	YGLDNFDTQFTSEPVQLTPDDEDAIKRIDQSEFEGFEYINPLLLSTE
PKCiota	538	FGLDNFDSQFTNEPVQLTPDDDDJVRKIDQSEFEGFEYINPLLMSAE
PKCdelta	628	RDYSNFDQEFLNEKARLSYSDKNLIDSMDQSAFAGFSFVNPKFEHLL
PKAgamma	323	GDASNFDDYEE-EELRISINEK-CAKEFSEF
PDK1	370	EDCYGNYDNLLSQFGCMQVSSSSSHSLSASDTGLPQRSGSNIEQYIHDLDSNSFELDLQ